Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1626GMS

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2		"Ask CAS" for self-help around the clock
NEWS 3	AUG 09	INSPEC enhanced with 1898-1968 archive
NEWS 4	AUG 28	ADISCTI Reloaded and Enhanced
NEWS 5	AUG 30	CA(SM)/CAplus(SM) Austrian patent law changes
NEWS 6	SEP 11	CA/CAplus enhanced with more pre-1907 records
NEWS 7	SEP 21	CA/CAplus fields enhanced with simultaneous left and right truncation
NEWS 8	SEP 25	CA(SM)/CAplus(SM) display of CA Lexicon enhanced
NEWS 9	SEP 25	CAS REGISTRY(SM) no longer includes Concord 3D coordinates
NEWS 10	SEP 25	CAS REGISTRY(SM) updated with amino acid codes for pyrrolysine
NEWS 11	SEP 28	CEABA-VTB classification code fields reloaded with new classification scheme
NEWS 12	OCT 19	LOGOFF HOLD duration extended to 120 minutes
NEWS 13	OCT 19	E-mail format enhanced
NEWS 14	OCT 23	Option to turn off MARPAT highlighting enhancements available
NEWS 15	OCT 23	CAS Registry Number crossover limit increased to 300,000 in multiple databases
NEWS 16	OCT 23	The Derwent World Patents Index suite of databases on STN has been enhanced and reloaded
NEWS 17	OCT 30	CHEMLIST enhanced with new search and display field
NEWS 18	NOV 03	JAPIO enhanced with IPC 8 features and functionality

NEWS EXPRESS	JUNE 30 CURRENT WINDOWS VERSION IS V8.01b, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 26 JUNE 2006.
NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8
NEWS X25	X.25 communication option no longer available

Enter NEWS followed by the item number or name to see news on that specific topic.

* * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 14:51:44 ON 05 NOV 2006

=>
Uploading
THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE
Do you want to switch to the Registry File?
Choice (Y/n):
Switching to the Registry File...
Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> FILE REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 14:51:59 ON 05 NOV 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 3 NOV 2006 HIGHEST RN 912441-38-4
DICTIONARY FILE UPDATES: 3 NOV 2006 HIGHEST RN 912441-38-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

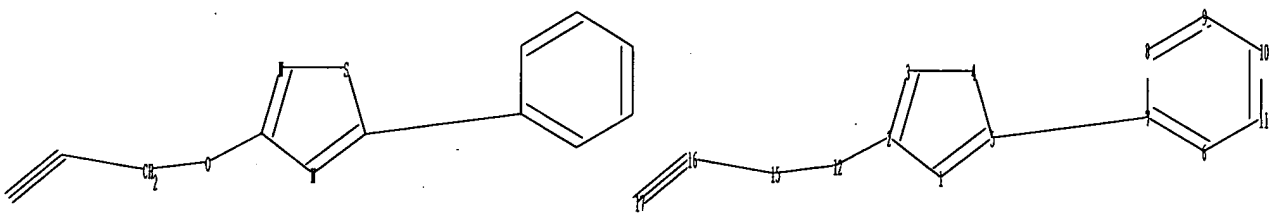
TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10530136d.str



chain nodes :
12 15 16 17
ring nodes :
1 2 3 4 5 6 7 8 9 10 11

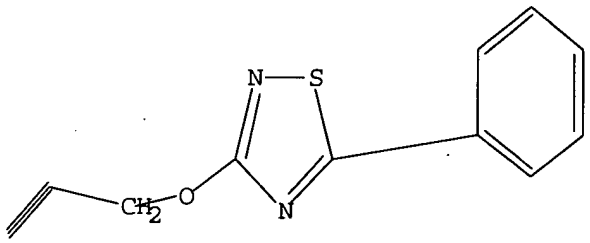
chain bonds :
2-12 5-7 12-15 15-16 16-17
ring bonds :
1-2 1-5 2-3 3-4 4-5 6-7 6-11 7-8 8-9 9-10 10-11
exact/norm bonds :
1-2 1-5 2-3 2-12 3-4
exact bonds :
4-5 5-7 12-15 15-16 16-17
normalized bonds :
6-7 6-11 7-8 8-9 9-10 10-11
isolated ring systems :
containing 1 : 6 :

G1:O,S,CH2,NH,Ak

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:CLASS 15:CLASS 16:CLASS 17:CLASS

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 O,S,CH2,NH,Ak

Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 14:52:12 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 4 TO ITERATE

100.0% PROCESSED 4 ITERATIONS 2 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 4 TO 200
PROJECTED ANSWERS: 2 TO 124

L2 2 SEA SSS SAM L1

=> s l1 sss full

FULL SEARCH INITIATED 14:52:18 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 70 TO ITERATE

100.0% PROCESSED 70 ITERATIONS 22 ANSWERS
SEARCH TIME: 00.00.01

L3 22 SEA SSS FUL L1

=> FIL HCAPLUS

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	166.94	167.15

FILE 'HCAPLUS' ENTERED AT 14:52:21 ON 05 NOV 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 5 Nov 2006 VOL 145 ISS 20
FILE LAST UPDATED: 3 Nov 2006 (20061103/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3
L4 1 L3

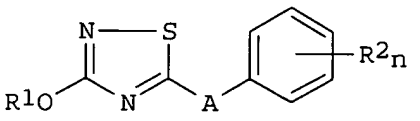
=> d l4 ibib abs hitstr tot

L4 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:900807 HCAPLUS
DOCUMENT NUMBER: 137:381259
TITLE: Preparation of 1,2,4-thiadiazole compounds and arthropodicides containing them
INVENTOR(S): Ihara, Hideki; Sakamoto, Noriyasu
PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002338557	A2	20021127	JP 2001-152269	20010522

WO 2004041798 A1 20040521 WO 2002-JP11644 20021108
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
AU 2002368330 A1 20040607 AU 2002-368330 20021108
BR 2002015911 A 20050726 BR 2002-15911 20021108
EP 1574505 A1 20050914 EP 2002-808100 20021108
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK
CN 1688559 A 20051026 CN 2002-829792 20021108
US 2006167266 A1 20060727 US 2005-530136 20050404
PRIORITY APPLN. INFO.: JP 2001-152269 A 20010522
WO 2002-JP11644 A 20021108

OTHER SOURCE(S): MARPAT 137:381259
GI

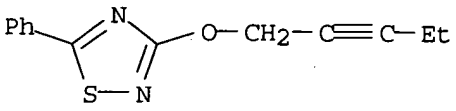


I

AB The compds. I [R1 = C3-7 (halo)alkenyl; R2 = halo, C1-4 alkyl, C1-3 haloalkyl, C1-4 haloalkoxy, cyano, NO2; n = 0-5; A = O, S,direct bond, CR3R4, NR5; R3, R4 = H, C1-4 alkyl; R5 = H, C1-7 alkyl, C1-3 haloalkyl, C2-4 (halo)alkoxyalkyl, C3-6 (halo)alkenyl, C3-7 (halo)alkynyl, CH2CN] and arthropod control agents containing I are claimed. A composition containing 5-phenyl-3-propargyloxy-1,2,4-thiadiazole (preparation given), showed ≥90% control against Aphis gossypii parasitic on cucumber seedlings.

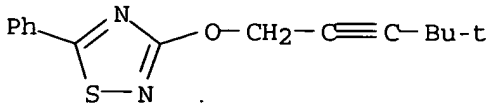
IT 476315-98-7 476315-99-8 476316-00-4
476316-01-5 476316-02-6 476316-03-7
476316-04-8 476316-05-9 476316-06-0
476316-07-1 476316-08-2 476316-09-3
476316-10-6 476316-11-7 476316-12-8
476316-13-9 476316-74-2
RL: AGR (Agricultural use); BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses)
(preparation of 1,2,4-thiadiazole compds. as arthropodicides)

RN 476315-98-7 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-pentynyloxy)-5-phenyl- (9CI) (CA INDEX NAME)

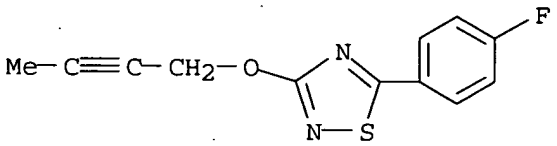


RN 476315-99-8 HCAPLUS

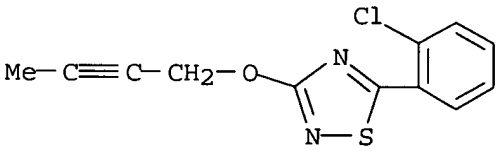
CN 1,2,4-Thiadiazole, 3-[(4,4-dimethyl-2-pentynyl)oxy]-5-phenyl- (9CI) (CA INDEX NAME)



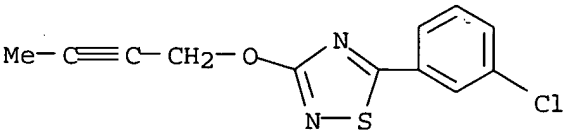
RN 476316-00-4 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(4-fluorophenyl)- (9CI) (CA INDEX NAME)



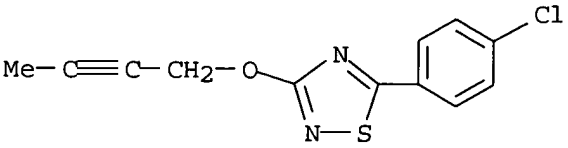
RN 476316-01-5 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(2-chlorophenyl)- (9CI) (CA INDEX NAME)



RN 476316-02-6 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(3-chlorophenyl)- (9CI) (CA INDEX NAME)

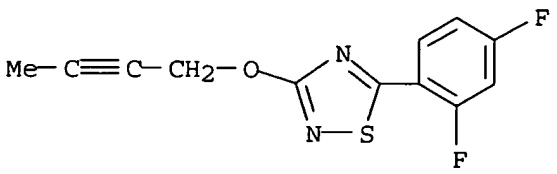


RN 476316-03-7 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(4-chlorophenyl)- (9CI) (CA INDEX NAME)

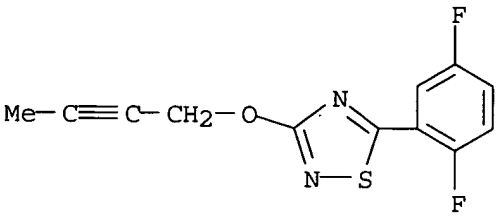


RN 476316-04-8 HCAPLUS

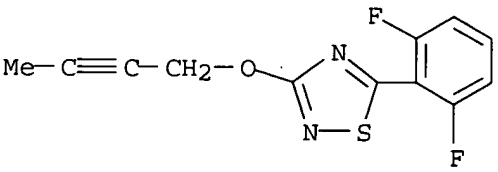
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(2,4-difluorophenyl)- (9CI) (CA INDEX NAME)



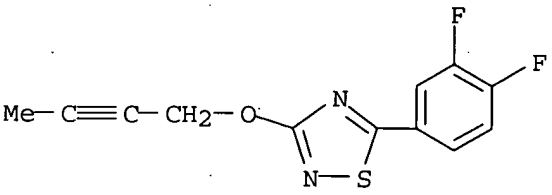
RN 476316-05-9 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(2,5-difluorophenyl)- (9CI) (CA INDEX NAME)



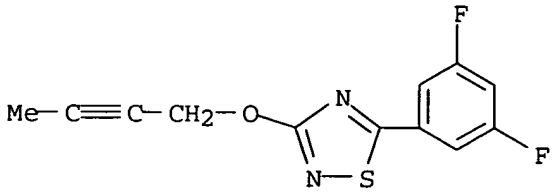
RN 476316-06-0 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(2,6-difluorophenyl)- (9CI) (CA INDEX NAME)



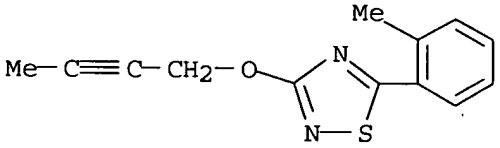
RN 476316-07-1 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(3,4-difluorophenyl)- (9CI) (CA INDEX NAME)



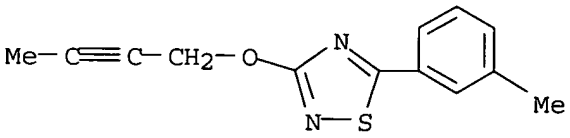
RN 476316-08-2 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(3,5-difluorophenyl)- (9CI) (CA INDEX NAME)



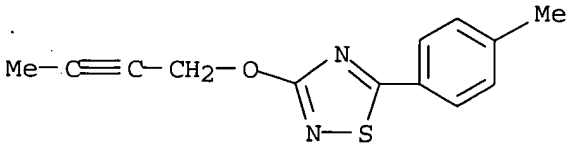
RN 476316-09-3 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(2-methylphenyl)- (9CI) (CA INDEX NAME)



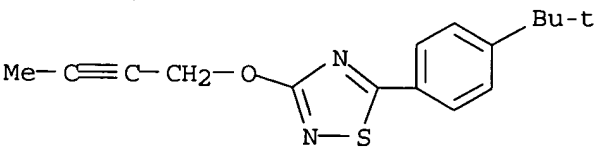
RN 476316-10-6 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(3-methylphenyl)- (9CI) (CA INDEX NAME)



RN 476316-11-7 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(4-methylphenyl)- (9CI) (CA INDEX NAME)

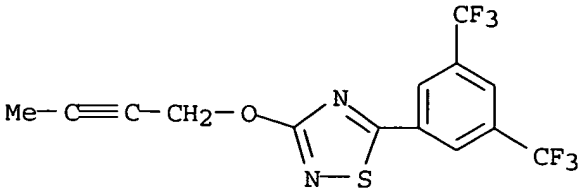


RN 476316-12-8 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-[4-(1,1-dimethylethyl)phenyl]- (9CI) (CA INDEX NAME)

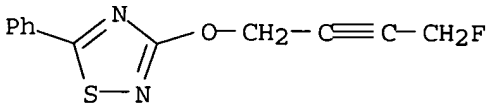


RN 476316-13-9 HCAPLUS
CN 1,2,4-Thiadiazole, 5-[3,5-bis(trifluoromethyl)phenyl]-3-(2-butynyloxy)-

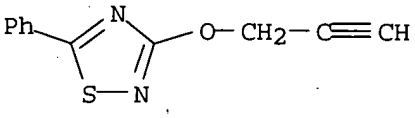
(9CI) (CA INDEX NAME)



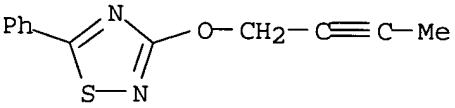
RN 476316-74-2 HCAPLUS
CN 1,2,4-Thiadiazole, 3-[(4-fluoro-2-butynyl)oxy]-5-phenyl- (9CI) (CA INDEX NAME)



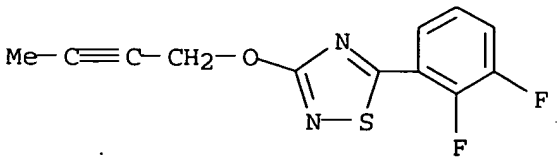
IT 476315-86-3P 476315-87-4P 476315-89-6P
476315-92-1P 476315-94-3P
RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 1,2,4-thiadiazole compds. as arthropodicides)
RN 476315-86-3 HCAPLUS
CN 1,2,4-Thiadiazole, 5-phenyl-3-(2-propynyloxy)- (9CI) (CA INDEX NAME)



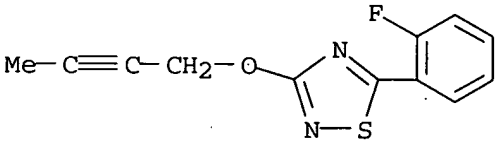
RN 476315-87-4 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-phenyl- (9CI) (CA INDEX NAME)



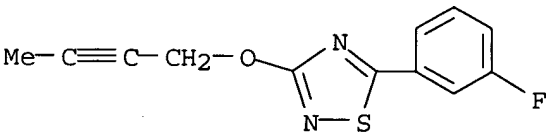
RN 476315-89-6 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(2,3-difluorophenyl)- (9CI) (CA INDEX NAME)



RN 476315-92-1 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(2-fluorophenyl)- (9CI) (CA INDEX NAME)



RN 476315-94-3 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(3-fluorophenyl)- (9CI) (CA INDEX NAME)



=> log y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	7.64	174.79
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.75	-0.75

STN INTERNATIONAL LOGOFF AT 14:52:38 ON 05 NOV 2006

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1626GMS

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2		"Ask CAS" for self-help around the clock
NEWS 3	AUG 09	INSPEC enhanced with 1898-1968 archive
NEWS 4	AUG 28	ADISCTI Reloaded and Enhanced
NEWS 5	AUG 30	CA(SM)/CAplus(SM) Austrian patent law changes
NEWS 6	SEP 11	CA/CAplus enhanced with more pre-1907 records
NEWS 7	SEP 21	CA/CAplus fields enhanced with simultaneous left and right truncation
NEWS 8	SEP 25	CA(SM)/CAplus(SM) display of CA Lexicon enhanced
NEWS 9	SEP 25	CAS REGISTRY(SM) no longer includes Concord 3D coordinates
NEWS 10	SEP 25	CAS REGISTRY(SM) updated with amino acid codes for pyrrolysine
NEWS 11	SEP 28	CEABA-VTB classification code fields reloaded with new classification scheme
NEWS 12	OCT 19	LOGOFF HOLD duration extended to 120 minutes
NEWS 13	OCT 19	E-mail format enhanced
NEWS 14	OCT 23	Option to turn off MARPAT highlighting enhancements available
NEWS 15	OCT 23	CAS Registry Number crossover limit increased to 300,000 in multiple databases
NEWS 16	OCT 23	The Derwent World Patents Index suite of databases on STN has been enhanced and reloaded
NEWS 17	OCT 30	CHEMLIST enhanced with new search and display field
NEWS 18	NOV 03	JAPIO enhanced with IPC 8 features and functionality

NEWS EXPRESS JUNE 30 CURRENT WINDOWS VERSION IS V8.01b, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 26 JUNE 2006.

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8
NEWS X25	X.25 communication option no longer available

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 08:33:21 ON 05 NOV 2006

=>
Uploading
THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE
Do you want to switch to the Registry File?
Choice (Y/n):
Switching to the Registry File...
Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> FILE REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 08:33:34 ON 05 NOV 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 3 NOV 2006 HIGHEST RN 912441-38-4
DICTIONARY FILE UPDATES: 3 NOV 2006 HIGHEST RN 912441-38-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

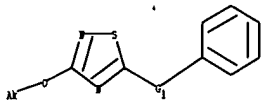
TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

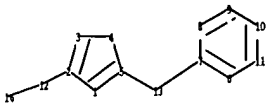
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10530136.str





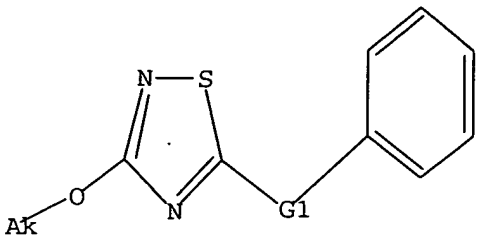
chain nodes :
12 13 16
ring nodes :
1 2 3 4 5 6 7 8 9 10 11
chain bonds :
2-12 5-13 7-13 12-16
ring bonds :
1-2 1-5 2-3 3-4 4-5 6-7 6-11 7-8 8-9 9-10 10-11
exact/norm bonds :
1-2 1-5 2-3 2-12 3-4 5-13 7-13 12-16
exact bonds :
4-5
normalized bonds :
6-7 6-11 7-8 8-9 9-10 10-11
isolated ring systems :
containing 1 : 6 :

G1:O,S,CH2,NH,Ak

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:CLASS 13:CLASS 16:CLASS

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 O,S,CH2,NH,Ak

Structure attributes must be viewed using STN Express query preparation.

```
=> s l1
SAMPLE SEARCH INITIATED 08:33:49 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -       99 TO ITERATE

100.0% PROCESSED       99 ITERATIONS                              3 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         1384 TO     2576
PROJECTED ANSWERS:               3 TO      163

L2            3 SEA SSS SAM L1

=> s l1 sss full
FULL SEARCH INITIATED 08:33:55 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     1861 TO ITERATE

100.0% PROCESSED     1861 ITERATIONS                             59 ANSWERS
SEARCH TIME: 00.00.01

L3            59 SEA SSS FUL L1

=> FIL HCAPLUS
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                              166.94     167.15

FILE 'HCAPLUS' ENTERED AT 08:34:02 ON 05 NOV 2006
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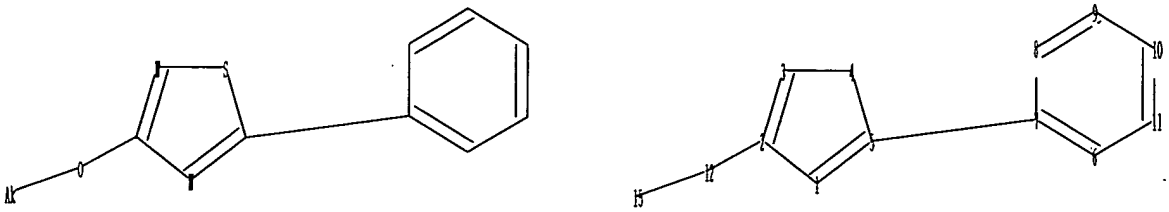
FILE COVERS 1907 - 5 Nov 2006 VOL 145 ISS 20
FILE LAST UPDATED: 3 Nov 2006 (20061103/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3
L4 13 L3

=>
Uploading C:\Program Files\Stnexp\Queries\10530136a.str



chain nodes :
12 15
ring nodes :
1 2 3 4 5 6 7 8 9 10 11
chain bonds :
2-12 5-7 12-15
ring bonds :
1-2 1-5 2-3 3-4 4-5 6-7 6-11 7-8 8-9 9-10 10-11
exact/norm bonds :
1-2 1-5 2-3 2-12 3-4 12-15
exact bonds :
4-5 5-7
normalized bonds :
6-7 6-11 7-8 8-9 9-10 10-11
isolated ring systems :
containing 1 : 6 :

G1:O,S,CH2,NH,Ak

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:CLASS 15:CLASS

L5 STRUCTURE UPLOADED

=> FIL REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	5.06	172.21

FILE 'REGISTRY' ENTERED AT 08:35:05 ON 05 NOV 2006

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 3 NOV 2006 HIGHEST RN 912441-38-4
DICTIONARY FILE UPDATES: 3 NOV 2006 HIGHEST RN 912441-38-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

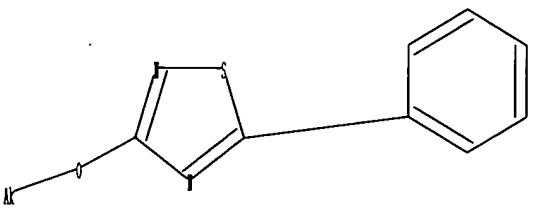
TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

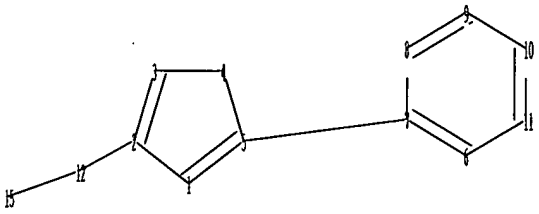
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10530136a.str





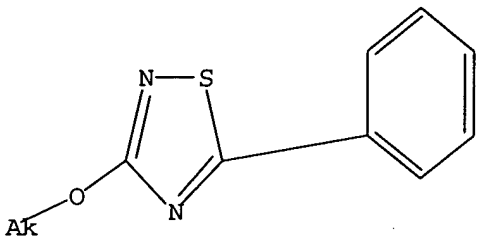
chain nodes :
12 15
ring nodes :
1 2 3 4 5 6 7 8 9 10 11
chain bonds :
2-12 5-7 12-15
ring bonds :
1-2 1-5 2-3 3-4 4-5 6-7 6-11 7-8 8-9 9-10 10-11
exact/norm bonds :
1-2 1-5 2-3 2-12 3-4 12-15
exact bonds :
4-5 5-7
normalized bonds :
6-7 6-11 7-8 8-9 9-10 10-11
isolated ring systems :
containing 1 : 6 :

G1:O,S,CH2,NH,Ak

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:CLASS 15:CLASS

L6 STRUCTURE UPLOADED

=> d l6
L6 HAS NO ANSWERS
L6 STR



G1 O,S,CH2,NH,Ak

Structure attributes must be viewed using STN Express query preparation.

=> s l6
SAMPLE SEARCH INITIATED 08:35:24 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 34 TO ITERATE

100.0% PROCESSED 34 ITERATIONS 8 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 331 TO 1029
PROJECTED ANSWERS: 8 TO 329

L7 8 SEA SSS SAM L6

=> s l6 sss full
FULL SEARCH INITIATED 08:35:31 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 521 TO ITERATE

100.0% PROCESSED 521 ITERATIONS 102 ANSWERS
SEARCH TIME: 00.00.01

L8 102 SEA SSS FUL L6

=> FIL HCAPLUS
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	166.94	339.15

FILE 'HCAPLUS' ENTERED AT 08:35:41 ON 05 NOV 2006
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FILE COVERS 1907 - 5 Nov 2006 VOL 145 ISS 20
FILE LAST UPDATED: 3 Nov 2006 (20061103/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

```
=> s l8
L9          14 L8

=> d his

     (FILE 'HOME' ENTERED AT 08:33:21 ON 05 NOV 2006)

     FILE 'REGISTRY' ENTERED AT 08:33:34 ON 05 NOV 2006
L1              STRUCTURE UPLOADED
L2            3 S L1
L3           59 S L1 SSS FULL

     FILE 'HCAPLUS' ENTERED AT 08:34:02 ON 05 NOV 2006
L4           13 S L3
L5              STRUCTURE UPLOADED

     FILE 'REGISTRY' ENTERED AT 08:35:05 ON 05 NOV 2006
L6              STRUCTURE UPLOADED
L7            8 S L6
L8          102 S L6 SSS FULL

     FILE 'HCAPLUS' ENTERED AT 08:35:41 ON 05 NOV 2006
L9           14 S L8

=> s l4 and py<=2002
      22829455 PY<=2002
L10         13 L4 AND PY<=2002

=> s l9 and py<=2002
      22829455 PY<=2002
L11         11 L9 AND PY<=2002

=> d l10 ibib abs hitstr tot

L10  ANSWER 1 OF 13  HCAPLUS  COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER:         2002:900807  HCAPLUS
DOCUMENT NUMBER:          137:381259
TITLE:                    Preparation of 1,2,4-thiadiazole compounds and
                          arthropodicides containing them
INVENTOR(S):              Ihara, Hideki; Sakamoto, Noriyasu
PATENT ASSIGNEE(S):       Sumitomo Chemical Co., Ltd., Japan
SOURCE:                   Jpn. Kokai Tokkyo Koho, 13 pp.
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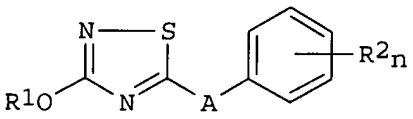
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002338557	A2	20021127	JP 2001-152269	20010522 <--
WO 2004041798	A1	20040521	WO 2002-JP11644	20021108
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002368330	A1	20040607	AU 2002-368330	20021108
BR 2002015911	A	20050726	BR 2002-15911	20021108
EP 1574505	A1	20050914	EP 2002-808100	20021108
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
CN 1688559	A	20051026	CN 2002-829792	20021108
US 2006167266	A1	20060727	US 2005-530136	20050404
PRIORITY APPLN. INFO.:			JP 2001-152269 A	20010522
			WO 2002-JP11644 A	20021108

OTHER SOURCE(S): MARPAT 137:381259
GI



I

AB The compds. I [R1 = C3-7 (halo)alkenyl; R2 = halo, C1-4 alkyl, C1-3 haloalkyl, C1-4 haloalkoxy, cyano, NO2; n = 0-5; A = O, S,direct bond, CR3R4, NR5; R3, R4 = H, C1-4 alkyl; R5 = H, C1-7 alkyl, C1-3 haloalkyl, C2-4 (halo)alkoxyalkyl, C3-6 (halo)alkenyl, C3-7 (halo)alkynyl, CH2CN] and arthropod control agents containing I are claimed. A composition containing 5-phenyl-3-propargyloxy-1,2,4-thiadiazole (preparation given), showed ≥90% control against Aphis gossypii parasitic on cucumber seedlings.

IT 476316-14-0 476316-15-1 476316-16-2
476316-17-3 476316-18-4 476316-19-5
476316-20-8 476316-21-9 476316-22-0
476316-23-1 476316-24-2 476316-25-3
476316-26-4 476316-27-5 476316-28-6
476316-29-7 476316-30-0 476316-31-1
476316-32-2 476316-33-3 476316-34-4
476316-35-5 476316-36-6 476316-37-7
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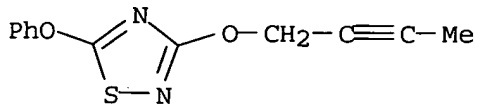
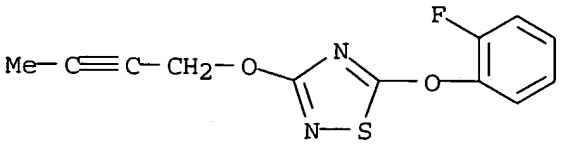
476316-41-3 476316-43-5 476316-45-7
476316-47-9 476316-49-1 476316-51-5

476316-53-7 476316-55-9 476316-57-1
476316-59-3 476316-70-8
RL: AGR (Agricultural use); BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses)
(preparation of 1,2,4-thiadiazole compds. as arthropodicides)

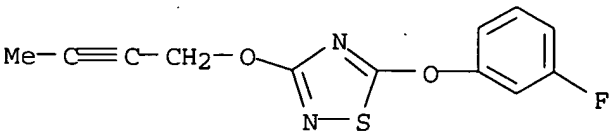
RN 476316-14-0 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-phenoxy- (9CI) (CA INDEX NAME)



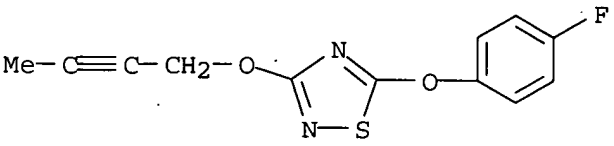
RN 476316-15-1 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(2-fluorophenoxy)- (9CI) (CA INDEX NAME)



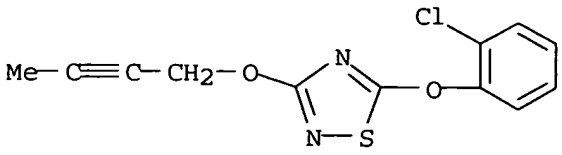
RN 476316-16-2 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(3-fluorophenoxy)- (9CI) (CA INDEX NAME)



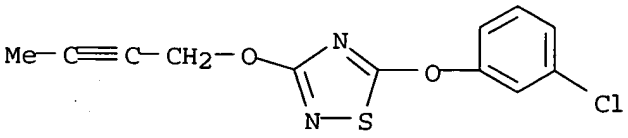
RN 476316-17-3 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(4-fluorophenoxy)- (9CI) (CA INDEX NAME)



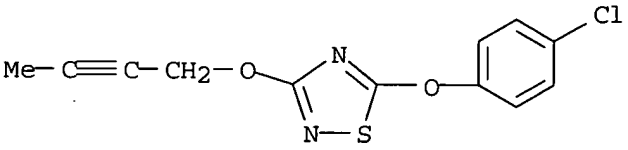
RN 476316-18-4 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(2-chlorophenoxy)- (9CI) (CA INDEX NAME)



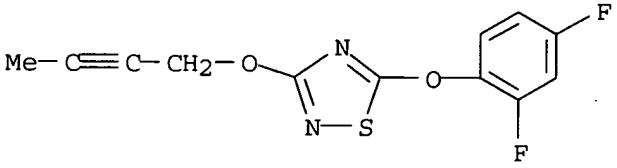
RN 476316-19-5 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(3-chlorophenoxy)- (9CI) (CA INDEX NAME)



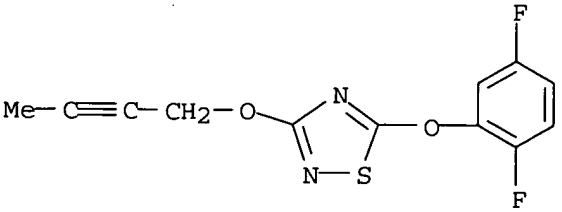
RN 476316-20-8 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(4-chlorophenoxy)- (9CI) (CA INDEX NAME)



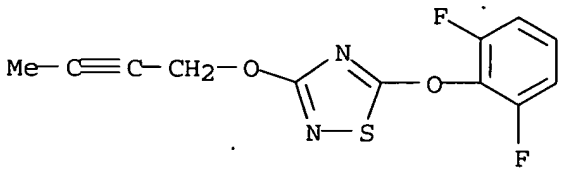
RN 476316-21-9 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(2,4-difluorophenoxy)- (9CI) (CA INDEX NAME)



RN 476316-22-0 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(2,5-difluorophenoxy)- (9CI) (CA INDEX NAME)



RN 476316-23-1 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(2,6-difluorophenoxy)- (9CI) (CA INDEX NAME)



RN 476316-24-2 HCAPLUS
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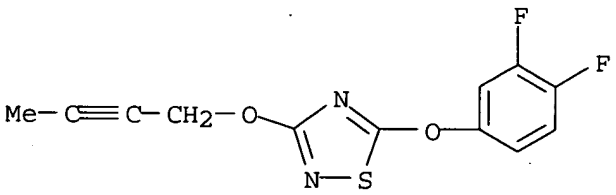
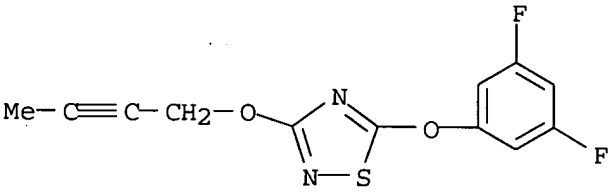
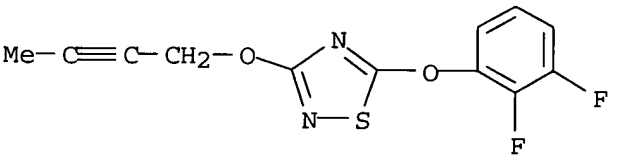


RN 476316-25-3 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(3,5-difluorophenoxy)- (9CI) (CA INDEX NAME)



RN 476316-26-4 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(2,3-difluorophenoxy)- (9CI) (CA INDEX NAME)



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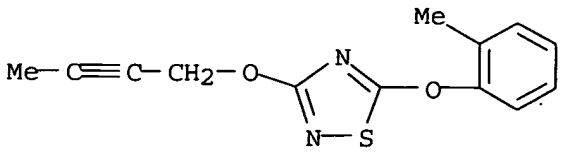

RN 476316-28-6 HCAPLUS
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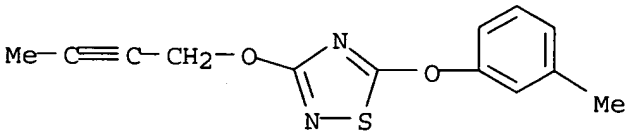

RN 476316-29-7 HCAPLUS
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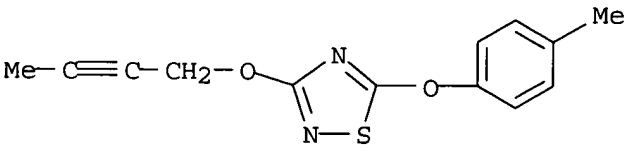

RN 476316-30-0 HCAPLUS
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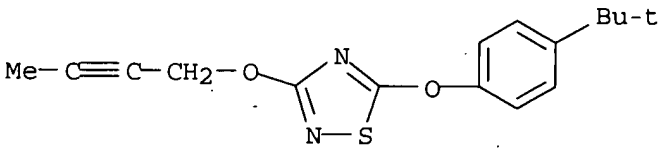

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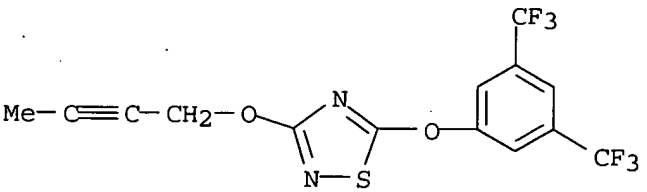
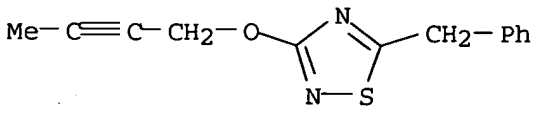
CN 1,2,4-Thiadiazole, 5-[3,5-bis(trifluoromethyl)phenoxy]-3-(2-butynyloxy)-(9CI) (CA INDEX NAME)

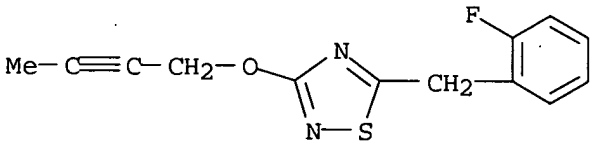


RN 476316-32-2 HCAPLUS

CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 476316-33-3 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-[(2-fluorophenyl)methyl]- (9CI) (CA INDEX NAME)



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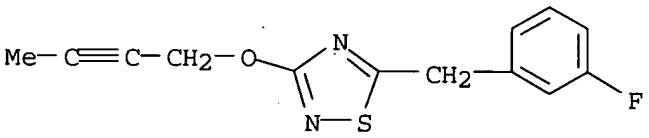
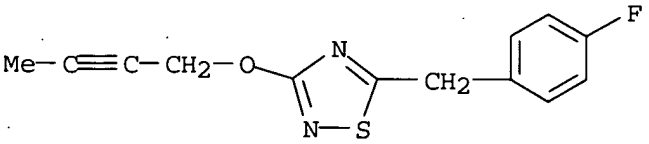
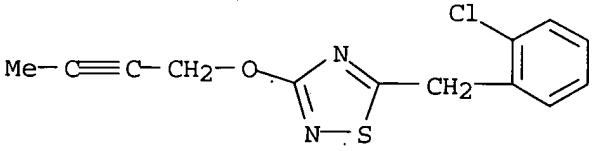
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-[(3-fluorophenyl)methyl]- (9CI) (CA INDEX NAME)



RN 476316-35-5 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-[(4-fluorophenyl)methyl]- (9CI) (CA INDEX NAME)

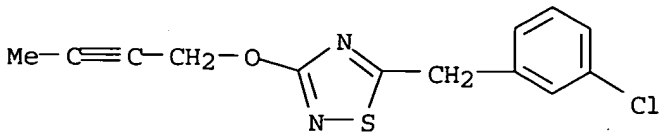


RN 476316-36-6 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-[(2-chlorophenyl)methyl]- (9CI) (CA INDEX NAME)

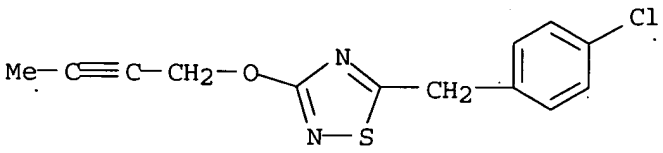


RN 476316-37-7 HCAPLUS

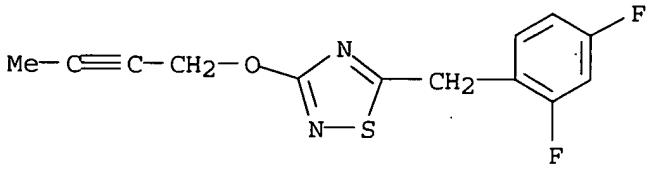
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-[(3-chlorophenyl)methyl]- (9CI) (CA INDEX NAME)



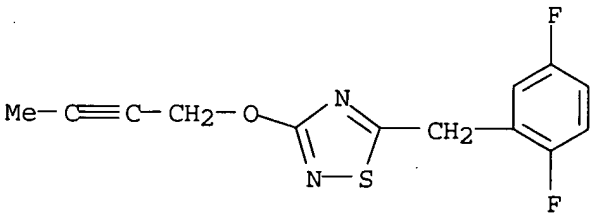
RN 476316-38-8 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-[(4-chlorophenyl)methyl]- (9CI) (CA INDEX NAME)



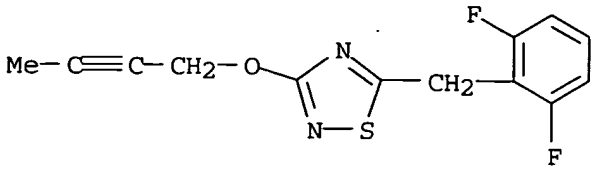
RN 476316-39-9 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-[(2,4-difluorophenyl)methyl]- (9CI) (CA INDEX NAME)



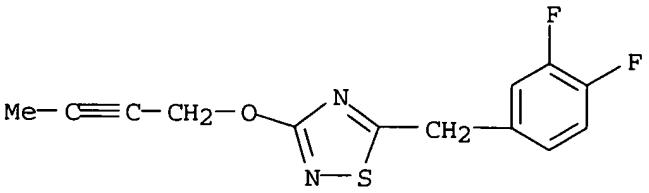
RN 476316-40-2 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-[(2,5-difluorophenyl)methyl]- (9CI) (CA INDEX NAME)



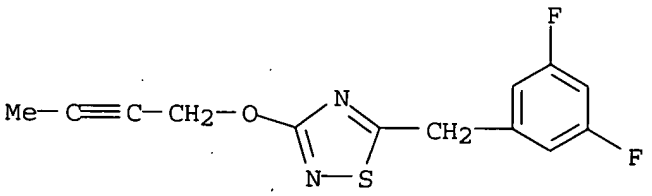
RN 476316-41-3 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-[(2,6-difluorophenyl)methyl]- (9CI) (CA INDEX NAME)



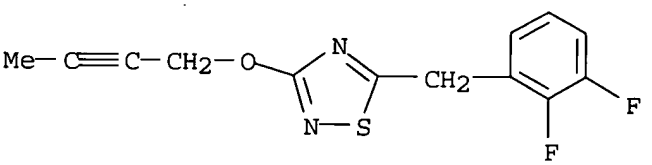
RN 476316-43-5 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-[(3,4-difluorophenyl)methyl]- (9CI) (CA INDEX NAME)



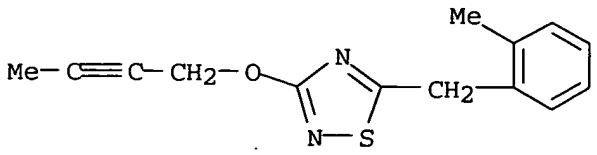
RN 476316-45-7 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-[(3,5-difluorophenyl)methyl]- (9CI) (CA INDEX NAME)



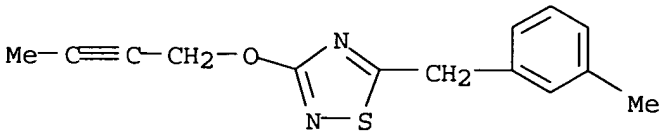
RN 476316-47-9 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-[(2,3-difluorophenyl)methyl]- (9CI) (CA INDEX NAME)



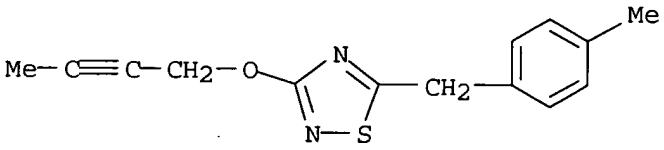
RN 476316-49-1 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-[(2-methylphenyl)methyl]- (9CI) (CA INDEX NAME)



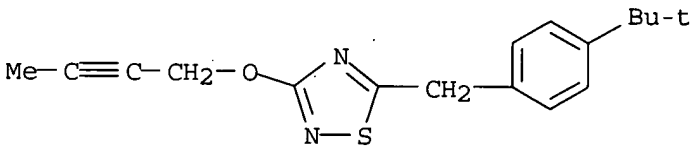
RN 476316-51-5 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-[(3-methylphenyl)methyl]- (9CI) (CA INDEX NAME)



RN 476316-53-7 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-[(4-methylphenyl)methyl]- (9CI) (CA INDEX NAME)



RN 476316-55-9 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-[[4-(1,1-dimethylethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)



RN 476316-57-1 HCAPLUS
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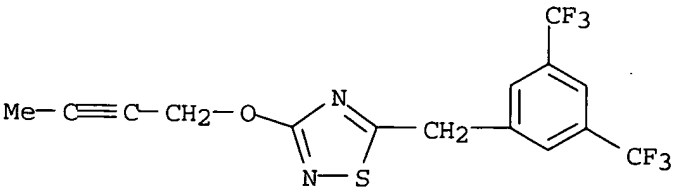
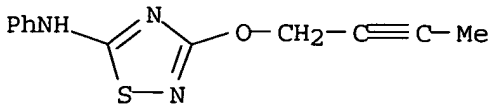
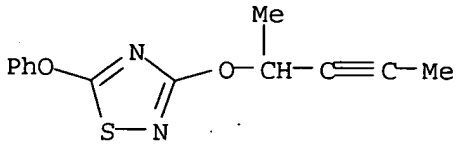


RN 476316-59-3 HCAPLUS

CN 1,2,4-Thiadiazol-5-amine, 3-(2-butynyloxy)-N-phenyl- (9CI) (CA INDEX NAME)



RN 476316-70-8 HCAPLUS
CN 1,2,4-Thiadiazole, 3-[(1-methyl-2-butynyl)oxy]-5-phenoxy- (9CI) (CA INDEX NAME)



L10 ANSWER 2 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:553541 HCAPLUS
DOCUMENT NUMBER: 133:163952
TITLE: Preparation of N2-phenylamidines as fungicides
INVENTOR(S): Charles, Mark David; Franke, Wilfried; Green, David Eric; Hough, Thomas Lawley; Mitchell, Dale Robert; Simpson, Donald James; Atherall, John Frederick
PATENT ASSIGNEE(S): Hoechst Schering Agrevo G.m.b.H., Germany
SOURCE: PCT Int. Appl., 76 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
WO 2000046184	A1	20000810	WO 2000-GB345	20000204	<--
W: AU, BR, CA, CN, CZ, HU, IL, IN, JP, KR, MX, RU, TR, UA, US, ZA					
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE					
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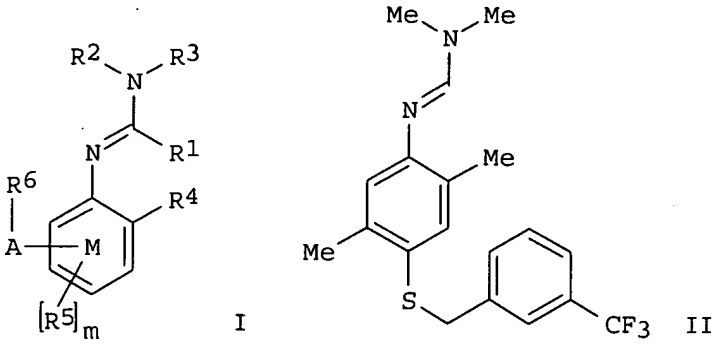
CA 2360943	C	20060418			
EP 1150944	A1	20011107	EP 2000-901791	20000204	<--
EP 1150944	B1	20030820			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI					
TR 200102237	T2	20011221	TR 2001-2237	20000204	<--
BR 2000009314	A	20020213	BR 2000-9314	20000204	<--
JP 2002536354	T2	20021029	JP 2000-597256	20000204	<--
AT 247629	E	20030915	AT 2000-901791	20000204	
AU 768156	B2	20031204	AU 2000-23088	20000204	
PT 1150944	T	20031231	PT 2000-901791	20000204	
ES 2200816	T3	20040316	ES 2000-901791	20000204	
RU 2234504	C2	20040820	RU 2001-124664	20000204	
US 6893650	B1	20050517	US 2001-890775	20000204	

ZA 2001005845	A	20021016	ZA 2001-5845		20010716 <--
HK 1043358	A1	20050506	HK 2002-105179		20020712
PRIORITY APPLN. INFO.:			GB 1999-2592	A	19990206
			WO 2000-GB345	W	20000204

OTHER SOURCE(S): MARPAT 133:163952
GI



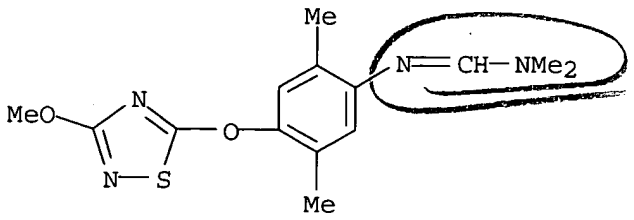
I II

AB The title compds. [I; R1 = alkyl, alkenyl, alkynyl, etc.; R2, R3 = R1, CN, acyl, etc.; R2 and R3, or R2 and R1, together with their interconnecting atoms may form (un)substituted ring; R4 = alkyl, alkenyl, alkynyl, etc.; m = 0-3; when present R5 = R4; R6 = (un)substituted carbo- or heterocyclyl; A = a direct bond, O, C.tplbond.C, etc.; AR6 and R5 together with benzene ring M form an (un)substituted fused ring system], useful as fungicides, were prepared E.g., a 3-step preparation of the formamidine II which showed moderate to total control against Erysiphe graminis f. sp. Tritici at 500 ppm (w/v) or less, was given.

IT 287939-10-0P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of N2-phenylamidines as fungicides)

RN 287939-10-0 HCAPLUS

CN Methanimidamide, N'-[4-[(3-methoxy-1,2,4-thiadiazol-5-yl)oxy]-2,5-dimethylphenyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

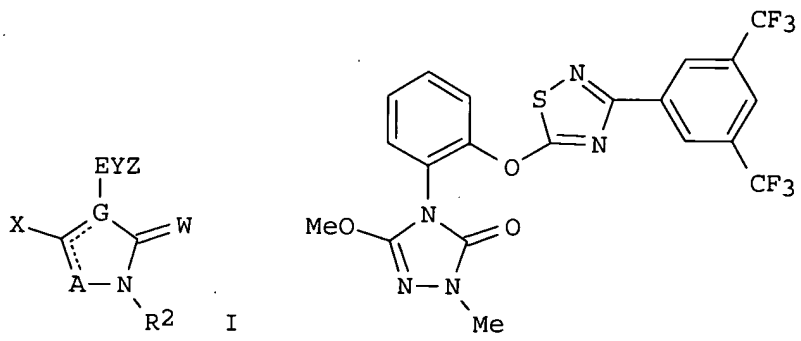
L10 ANSWER 3 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:385479 HCAPLUS

DOCUMENT NUMBER: 129:54375
TITLE: Arthropodicidal and fungicidal cyclic amides [triazolones] and their preparation, use, and compositions
INVENTOR(S): Brown, Richard James; Chan, Dominic Ming-Tak; Howard, Michael Henry, Jr.; Daniel, Dilon Jancey; Clark, David Alan; Selby, Thomas Paul
PATENT ASSIGNEE(S): E. I. Du Pont de Nemours & Co., USA
SOURCE: PCT Int. Appl., 232 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9823155	A1	19980604	WO 1996-US18916	19961126 <--
W: JP, KR				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
ZA 9709943	A	19990505	ZA 1997-9943	19971105 <--
WO 9823156	A1	19980604	WO 1997-US21944	19971125 <--
W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GE, HU, ID, IL, IS, JP, KG, KP, KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, SL, TJ, TM, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9854633	A1	19980622	AU 1998-54633	19971125 <--
EP 944314	A1	19990929	EP 1997-948597	19971125 <--
R: CH, DE, DK, ES, FR, GB, IT, LI, NL, IE				
BR 9713415	A	20000418	BR 1997-13415	19971125 <--
JP 2001506984	T2	20010529	JP 1998-524889	19971125 <--
MX 9904789	A	20000131	MX 1999-4789	19990524 <--
KR 2000057254	A	20000915	KR 1999-704639	19990526 <--

PRIORITY APPLN. INFO.:			
	WO 1996-US18916	A	19961126
	US 1996-33614P	P	19961219
	US 1997-48844P	P	19970606
	WO 1997-US21944	W	19971125

OTHER SOURCE(S): MARPAT 129:54375
GI



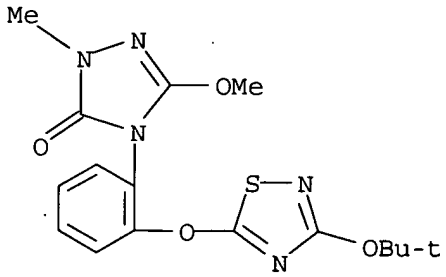
I II

AB Title compds. I and their N-oxides and agriculturally suitable salts are disclosed [wherein E = (un)substituted 1,2-phenylene, naphthalene or heterocyclyl; A = O, S, N, NR3 or CR4; G = C or N; when G is C, then A is O, S or NR3 and the floating double bond is attached to G; and when G is N, than A is N or CR4 and the floating double bond is attached to A; W = O, S, NH, N(C1-C6 alkyl) or NO(C1-C6 alkyl); X = H, OR1, SOmR1, halo, C1-C6 alkyl, C1-C6 haloalkyl, C3-C6 cycloalkyl, cyano, NH2, NHR1, N(C1-C6 alkyl)R1, NH(C1-C6 alkoxy) or N(C1-C6 alkoxy)R1; R2 = H, C1-C6 alkyl, C1-C6 haloalkyl, C2-C6 haloalkyl, C2-C6 alkenyl, C2-C6 haloalkenyl, C2-C6 alkynyl, C2-C6 haloalkynyl, C3-C6 cycloalkyl, C2-C4 alkylcarbonyl, C2-C6 alkoxycarbonyl, hydroxy, C1-C2 alkoxy, or acetyloxy; R1= (halo)alkyl, (halo)alkenyl, etc.; R3= H, (halo)alkyl, etc.; Y = O, CO, SO, etc.; Z = (un)substituted alkyl, alkenyl or alkynyl, R4 = H, halo, alkyl, etc.; m = 0, 1 or 2]. Claims cover methods of arthropod and fungal control, novel compds., arthropodicidal and fungicidal compns., and novel intermediates. Approx. 1000 invention compds. were prepared For instance, 5-chloro-2,4-dihydro-4-(2-methoxyphenyl)-2-methyl-3H-1,2,4-triazol-3-one (preparation given) underwent a sequence of cleavage of the Me ether with BBr3, methoxylation of the chloride with NaOMe, and etherification of the phenolic hydroxy group with 5-chloro-3-[3,5-bis(trifluoromethyl)phenyl]-1,2,4-thiadiazole, to give title compound II. Selected I were active in screens against Erysiphe graminis, Pyricularia oryzae, Spodoptera frugiperda, Tetranychus urticae, and a variety of other standard pests.

IT 208528-37-4P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation as arthropodicide and fungicide)

RN 208528-37-4 HCAPLUS

CN 3H-1,2,4-Triazol-3-one, 4-[2-[[3-(1,1-dimethylethoxy)-1,2,4-thiadiazol-5-yl]oxy]phenyl]-2,4-dihydro-5-methoxy-2-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

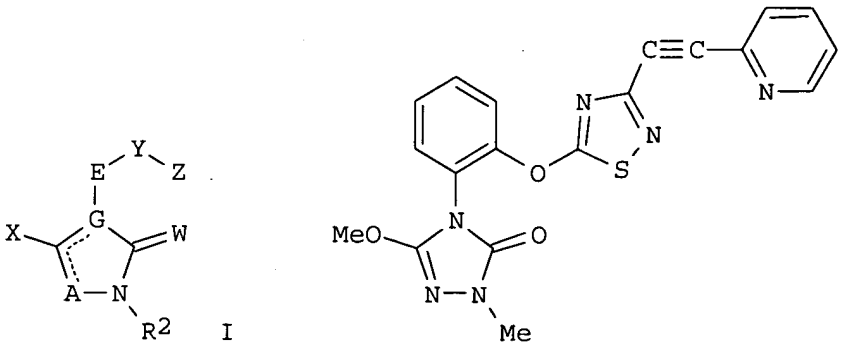
L10 ANSWER 4 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:112354 HCAPLUS
DOCUMENT NUMBER: 128:167436
TITLE: Preparation of arthropodicidal and fungicidal cyclic amides
INVENTOR(S): Brown, Richard James; Chan, Dominic Ming-Tak; Clark, David Alan; Drumm, Joseph Eugene, III; Koether, Gerard Michael; McCann, Stephen Frederick; Rorer, Morris Padgett; Selby, Thomas Paul; Walker, Michael Paul

PATENT ASSIGNEE(S): E. I. Du Pont de Nemours & Co., USA; Brown, Richard James; Chan, Dominic Ming-Tak; Clark, David Alan; Drumm, Joseph Eugene, III; Koether, Gerard Michael; McCann, Stephen Frederick; Rorer, Morris Padgett; Selby, Thomas Paul; Walker, Michael Paul
SOURCE: PCT Int. Appl., 130 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9805652	A2	19980212	WO 1997-US12809	19970724 <--
W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GE, HU, IL, IS, JP, KG, KP, KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, SL, TJ, TM, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9738890	A1	19980225	AU 1997-38890	19970724 <--
EP 934283	A2	19990811	EP 1997-936152	19970724 <--
R: DE, FR, GB, IT				
BR 9711816	A	19990831	BR 1997-11816	19970724 <--
CN 1231663	A	19991013	CN 1997-198356	19970724 <--
JP 2000516583	T2	20001212	JP 1998-507942	19970724 <--
MX 9901173	A	20000131	MX 1999-1173	19990201 <--

PRIORITY APPLN. INFO.:	US 1996-22933P	P	19960801
	WO 1997-US12809	W	19970724

OTHER SOURCE(S): MARPAT 128:167436
GI



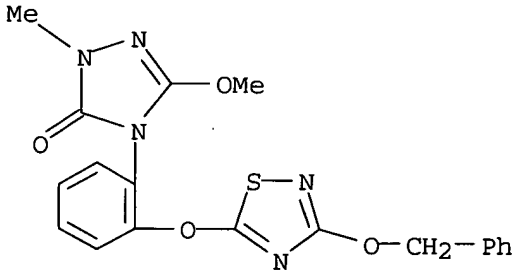
AB The title compds. [I; E = (un)substituted 1,2-phenylene, naphthalene, 5-12 membered monocyclic and fused bicyclic heteroaryl; A = O, S, N, NR5, CR14; G = C, N (provided that when G = C, then A = O, S, NR5 and the floating double bond is attached to G; and when G = N, then A = N, CR14 and the floating double bond is attached to A); W = O, S, NH, N(C1-6alkyl), NO(C1-6alkyl); X = OR1, S(O)mR1, halo; Y = O, S(O)n, NR15, etc.; Z = (un)substituted C3-8 cycloalkyl, C3-8 cycloalkenyl, Ph, etc.; R1 = C1-6

alkyl, C1-6 haloalkyl, C2-6 alkenyl, etc.; R2 = H, C1-6 alkyl, C1-6 haloalkyl, etc.; R5 = H, C1-6 alkyl, C1-6 haloalkyl, etc.; R14 = H, halo, C1-6 alkyl, etc.; R15 = H, C1-3 alkyl, C3-6 cycloalkyl, etc.; m, n = 0-2], useful for controlling plant diseases caused by fungal plant pathogens, and for controlling arthropods, were prepared Thus, reaction of 2,4-dihydro-4-(2-hydroxyphenyl)-5-methoxy-2-methyl-3H-1,2,4-triazol-3-one with 3-iodo-5-(methylsulfonyl)-1,2,4-thiadiazole in the presence of K2CO3 in Me2CO followed by reacting the resulting 2,4-dihydro-4-{2-[(3-iodo-1,2,4-thiadiazol-5-yl)oxy]phenyl}-5-methoxy-2-methyl-3H-1,2,4-triazol-3-one with 2-ethynylpyridine in the presence of CuI, PdCl2(PPh3)2 and Et3N in DMF afforded the title compound II which showed 95% control against Erypsiphe graminis (the causal agent of wheat powdery mildew) at 500 g/ha.

IT 203054-02-8P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of arthropodicidal and fungicidal cyclic amides)

RN 203054-02-8 HCAPLUS

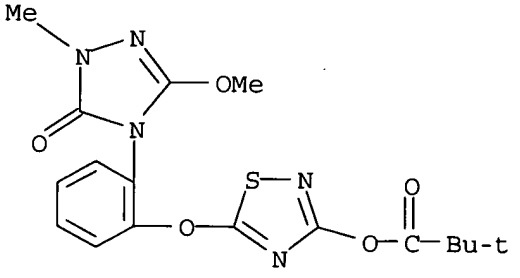
CN 3H-1,2,4-Triazol-3-one, 2,4-dihydro-5-methoxy-2-methyl-4-[2-[[3-(phenylmethoxy)-1,2,4-thiadiazol-5-yl]oxy]phenyl]- (9CI) (CA INDEX NAME)



IT 203053-62-7P 203053-63-8P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of arthropodicidal and fungicidal cyclic amides)

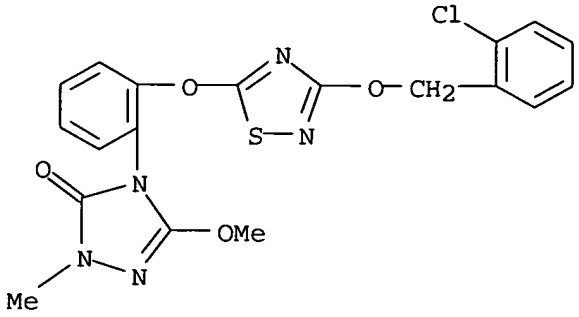
RN 203053-62-7 HCAPLUS

CN Propanoic acid, 2,2-dimethyl-, 5-[2-(1,5-dihydro-3-methoxy-1-methyl-5-oxo-4H-1,2,4-triazol-4-yl)phenoxy]-1,2,4-thiadiazol-3-yl ester (9CI) (CA INDEX NAME)

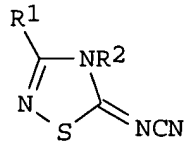


RN 203053-63-8 HCAPLUS

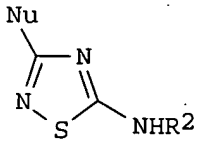
CN 3H-1,2,4-Triazol-3-one, 4-[2-[[3-[(2-chlorophenyl)methoxy]-1,2,4-thiadiazol-5-yl]oxy]phenyl]-2,4-dihydro-5-methoxy-2-methyl- (9CI) (CA INDEX NAME)



L10 ANSWER 5 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:264061 HCAPLUS
DOCUMENT NUMBER: 122:239609
TITLE: Boulton-Katritzky rearrangement of 5-(cyanoimino)-1,2,4-thiadiazolines
AUTHOR(S): Sonnenschein, Helmut; Schmitz, Ernst; Gruendemann, Egon; Schroeder, Edith
CORPORATE SOURCE: Inst. Angewandte Chem., Berlin, D-12484, Germany
SOURCE: Liebigs Annalen der Chemie (1994), (12), 1177-80
CODEN: LACHDL; ISSN: 0170-2041
PUBLISHER: VCH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 122:239609
GI



I



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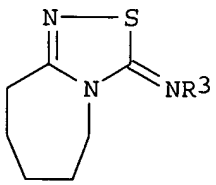
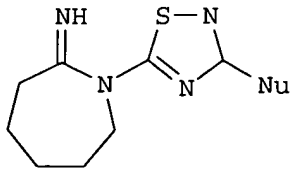


III



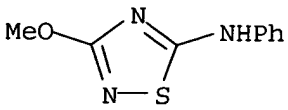
IV

AB The products of the addition of nucleophiles (alcs., amines) to the cyano group of 5-(cyanoimino)thiadiazolines I (R1 = Ph, Me, R2 = Ph, 2,6-Cl2C6H3, 3-MeC6H4, Me, Me2CHCH2) undergo a Boulton-Katritzky rearrangement. The thiadiazoles II (Nu = OMe, NMe2) are formed by subsequent nitrile elimination. In the case of bicyclic

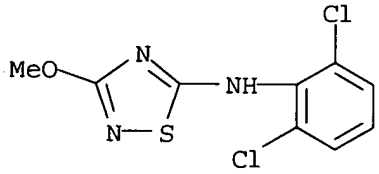
thiadiazoloazepine III (R3 = cyano), an equilibrium mixture of unrearranged iminothiadiazoline III (R3 = CR4:NH, R4 = OMe, NMe2) and rearranged thiadiazole IV is obtained as an intermediate.

IT 90564-94-6P 162231-59-6P 162231-61-0P
162231-71-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(Boulton-Katritzky rearrangement of (cyanoimino)thiadiazolines)

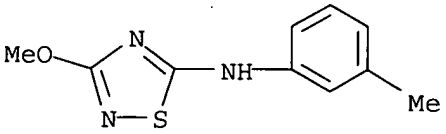
RN 90564-94-6 HCAPLUS
CN 1,2,4-Thiadiazol-5-amine, 3-methoxy-N-phenyl- (9CI) (CA INDEX NAME)



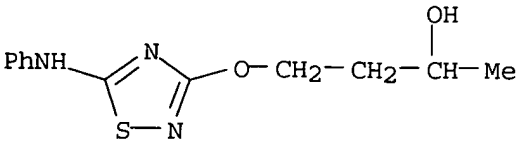
RN 162231-59-6 HCAPLUS
CN 1,2,4-Thiadiazol-5-amine, N-(2,6-dichlorophenyl)-3-methoxy- (9CI) (CA INDEX NAME)



RN 162231-61-0 HCAPLUS
CN 1,2,4-Thiadiazol-5-amine, 3-methoxy-N-(3-methylphenyl)- (9CI) (CA INDEX NAME)



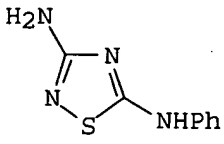
RN 162231-71-2 HCAPLUS
CN 2-Butanol, 4-[[5-(phenylamino)-1,2,4-thiadiazol-3-yl]oxy]- (9CI) (CA INDEX NAME)

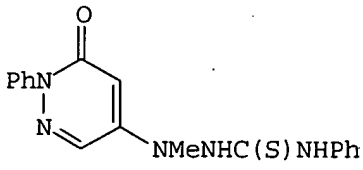


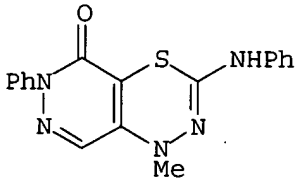
L10 ANSWER 6 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:122298 HCAPLUS
DOCUMENT NUMBER: 114:122298
TITLE: Oxidative heterocyclization using diethyl

azodicarboxylate

AUTHOR(S): Kihara, Yoshito; Kabashima, Shigeru; Uno, Kazue; Okawara, Tadashi; Yamasaki, Tetsuo; Furukawa, Mitsuru
CORPORATE SOURCE: Fac. Pharm. Sci., Kumamoto Univ., Kumamoto, 862, Japan
SOURCE: Synthesis (1990), (11), 1020-3
CODEN: SYNTBF; ISSN: 0039-7881
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 114:122298
GI


II

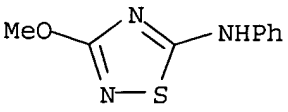

III


IV

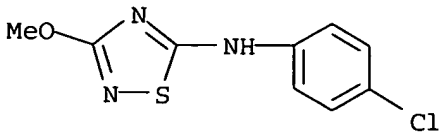
AB The reactions of amidinothioureas, imidoylthioureas, thioacylamidines, O-methyl-1-aryl-2-thioisobiurets, and 1-arylisodithiobiurets with di-Et azodicarboxylate (I) gave the corresponding thiadiazoles by the oxidative cyclic S-N bond formation. Thus, H2NC(:NH)NHC(S)NHPh was treated with I in EtOH to give 70% thiadiazole II. Analogously, the oxidative cyclization of 2-phenyl-5-(1-methylthiosemicarbazido)-3(2H)-pyridazinones, e.g., III, with I provided 4-methyl-7-phenyl-4H-pyridazino[4,5-e][1,3,4]thiadiazin-8(7H)-ones, e.g., IV.

IT 90564-94-6P 132533-37-0P 132533-38-1P
132533-39-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

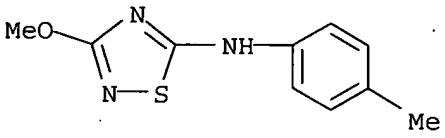
RN 90564-94-6 HCAPLUS
CN 1,2,4-Thiadiazol-5-amine, 3-methoxy-N-phenyl- (9CI) (CA INDEX NAME)



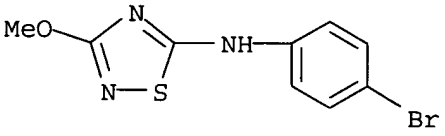
RN 132533-37-0 HCAPLUS
CN 1,2,4-Thiadiazol-5-amine, N-(4-chlorophenyl)-3-methoxy- (9CI) (CA INDEX NAME)



RN 132533-38-1 HCAPLUS
CN 1,2,4-Thiadiazol-5-amine, 3-methoxy-N-(4-methylphenyl)- (9CI) (CA INDEX NAME)



RN 132533-39-2 HCAPLUS
CN 1,2,4-Thiadiazol-5-amine, N-(4-bromophenyl)-3-methoxy- (9CI) (CA INDEX NAME)



L10 ANSWER 7 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1986:626588 HCAPLUS
DOCUMENT NUMBER: 105:226588
TITLE: 1,2,4-Thiadiazole derivatives
INVENTOR(S): Takiguchi, Daigaku; Kano, Saburo
PATENT ASSIGNEE(S): Nippon Soda Co., Ltd., Japan
SOURCE: PCT Int. Appl., 60 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

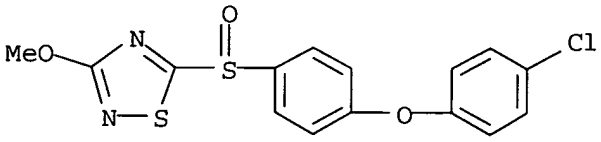
PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 8602927	A1	19860522	WO 1985-JP617		19851106 <--
W: AU, BR, DK, FI, JP, KR, NO, US					
RW: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE					
AU 8550679	A1	19860603	AU 1985-50679		19851106 <--
PRIORITY APPLN. INFO.:			JP 1984-234215	A	19841108
			WO 1985-JP617	A	19851106

GI For diagram(s), see printed CA Issue.
AB The title compds. [I; R = Q, Q1, Q2; R1 = H, halo, alkyl, CF3C, Ph, alkoxy; n = 0-2; R2 = halo, (halo)alkyl; m = 0-2; R3 = aryl; X, X1, X2 = CH, N, N(O); Z = O, CO, NHCO, NH, alkylene, etc.; X3 = O, CH2, S, S(O)2; X4 = (CH2)4, CH:CHCH:CH; R4, R5 = H, halo, alkyl], useful as fungicides

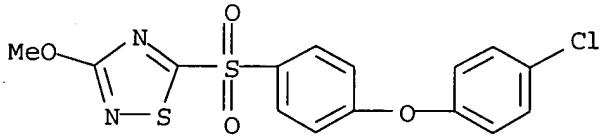
and protozoacides, were prepared Thus, a mixture of QSH (R2m = H; ZR3 = OPh-p; X = CH) and 5-Bromo-1,2,4-thiadiazole in EtOH containing NaOMe was stirred for 1/2 h in an ice bath and then heated at 50° for 2 h to give 94% I (I; R = Q; R2m = H; ZR3 = OPh-p; n = 0), whose oxidation with m-ClC6H5C(O)OOH gave 67.4% I (I; R = Q; R2m = H; ZR3 = OPh-p; n = 2). I at 0.625-1.25 μg/mL were active against Trichophyton mentagrophytes and Candida albicans.

IT 105422-76-2P 105422-77-3P 105422-90-0P
105422-91-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as fungicide and protozoacide)

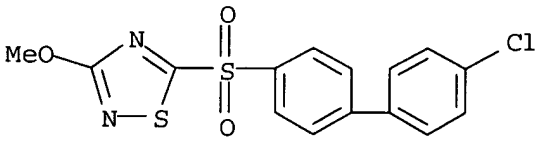
RN 105422-76-2 HCAPLUS
CN 1,2,4-Thiadiazole, 5-[[4-(4-chlorophenoxy)phenyl]sulfinyl]-3-methoxy-(9CI) (CA INDEX NAME)



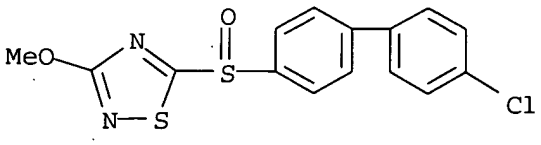
RN 105422-77-3 HCAPLUS
CN 1,2,4-Thiadiazole, 5-[[4-(4-chlorophenoxy)phenyl]sulfonyl]-3-methoxy-(9CI) (CA INDEX NAME)



RN 105422-90-0 HCAPLUS
CN 1,2,4-Thiadiazole, 5-[(4'-chloro[1,1'-biphenyl]-4-yl)sulfonyl]-3-methoxy-(9CI) (CA INDEX NAME)



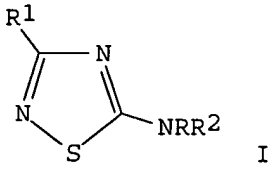
RN 105422-91-1 HCAPLUS
CN 1,2,4-Thiadiazole, 5-[(4'-chloro[1,1'-biphenyl]-4-yl)sulfinyl]-3-methoxy-(9CI) (CA INDEX NAME)



L10 ANSWER 8 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1985:615296 HCAPLUS
DOCUMENT NUMBER: 103:215296
TITLE: 3-Substituted 5-amino-1,2,4-thiadiazoles
INVENTOR(S): Martin, Dieter; Graubaum, Heinz
PATENT ASSIGNEE(S): Akademie der Wissenschaften der DDR, Ger. Dem. Rep.
SOURCE: Ger. (East), 13 pp.
CODEN: GEXXA8
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DD 217517	A1	19850116	DD 1983-250233	19830427 <--
PRIORITY APPLN. INFO.:			DD 1983-250233	19830427

OTHER SOURCE(S): CASREACT 103:215296
GI

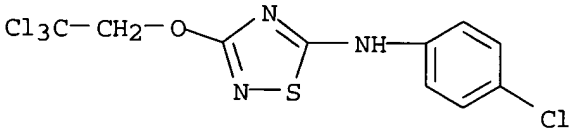


I

AB Thiadiazoles I [R = H, alkyl, (un)substituted aryl; R1 = CCl3, alkoxy, (un)substituted aryloxy; R2 = H, C(:NH)R1], useful as antimalarials and agricultural fungicides, herbicides, bactericides, algicides, nematocides and nitrification inhibitors (no data), were prepared by 5 methods. 5-Aminothiatriazole in an inert organic solvent was treated with PhOCN with stirring at 0-20°, then at room temperature after cessation of N evolution to give 60% I (R = R2 = H, R1 = PhO).

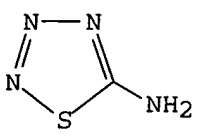
IT 94295-69-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as antimalarial and pesticide)

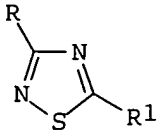
RN 94295-69-9 HCAPLUS
CN 1,2,4-Thiadiazol-5-amine, N-(4-chlorophenyl)-3-(2,2,2-trichloroethoxy)-(9CI) (CA INDEX NAME)



L10 ANSWER 9 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1985:504890 HCAPLUS
DOCUMENT NUMBER: 103:104890
TITLE: Synthesis of 1,2,4-thiadiazoles with potential fungistatic properties

AUTHOR(S): Martin, D.; Graubaum, H.
CORPORATE SOURCE: Cent. Inst. Org. Chem., Ger. Acad. Sci., Berlin, DDR-1199, Ger. Dem. Rep.
SOURCE: Tagungsbericht - Akademie der Landwirtschaftswissenschaften der Deutschen Demokratischen Republik (1984), 222(Syst. Fungic. Antifungal Compd.), 341-5
CODEN: TALDA3; ISSN: 0138-2659
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 103:104890
GI


I

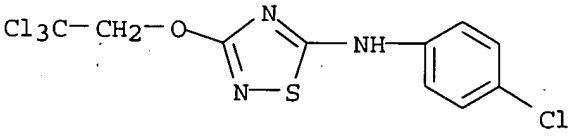

II

AB Treating aminothiatriazole I with RCN (R = PhO, 2-ClC6H4O, 3-, 4-MeC6H4O, 4-MeOC6H4O, Cl3C) gave 39-92% II (R1 = NH2) which at 30° react further to give amidines II [R1 = NHC(:NH)R]. Treating [alkyl(aryl)amino]thiatriazoles with RCN (R as above) gave II [R1 = NR2C(:NH)R, R2 = alkyl, aryl] which are converted to piperidino or morpholino derivs.

IT 94295-69-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

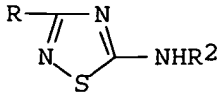
RN 94295-69-9 HCAPLUS

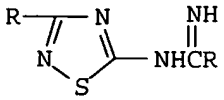
CN 1,2,4-Thiadiazol-5-amine, N-(4-chlorophenyl)-3-(2,2,2-trichloroethoxy)-(9CI) (CA INDEX NAME)

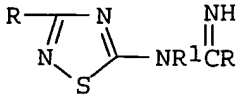


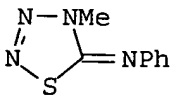
L10 ANSWER 10 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1985:166666 HCAPLUS
DOCUMENT NUMBER: 102:166666
TITLE: Cyanic acid esters. 36. 1,2,4-Thiadiazoles from amino-1,2,3,4-thiatriazoles and cyano compounds
AUTHOR(S): Martin, Dieter; Graubaum, Heinz; Kulpe, Siegfried
CORPORATE SOURCE: Cent. Inst. Org. Chem., Acad. Sci., Berlin, DDR-1199, Ger. Dem. Rep.
SOURCE: Journal of Organic Chemistry (1985), 50(8), 1295-8
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English

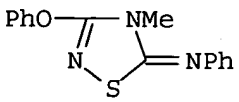
OTHER SOURCE(S): CASREACT 102:166666
GI


II, R^2=H
VI, R^2=R^1


III


V


VII

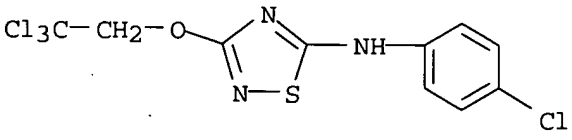

VIII

AB 5-Amino-1,2,3,4-thiatriazole (I) reacted with aryl cyanates RCN[R = R1C6H4O(R1 = H, 2-Cl, 3-Me, 4-MeO)] or Cl3CCN at 0° to give 3-substituted 5-amino-1,2,4-thiadiazoles II in yields of 39-92%. Using 2 equiv of aryl cyanate at temps. .apprx.40° gave 5-(iminocarbonylamino)-1,2,4-thiadiazoles III. In contrast to I, 5-alkyl(aryl)amino-1,2,3,4-thiatriazoles (IV) reacted with nitriles to give only 5-(iminocarbonylamino)-1,2,4-thiadiazoles V (R = PhO, 4-MeOC6H4O, 2,4-Cl2C6H3O, Cl3CCH2O, 4-MeC6H4O; R1 = Me, Et, Bu, Ph, 4-ClC6H4; 4-FC6H4, 4-MeC6H4). Deacylation of V with secondary amines gave 5-alkyl(aryl)amino-1,2,4-thiadiazoles VI (R = 4-MeOC6H4O, Cl3CCH2O, PhO, Cl3C; R1 = Ph, 4-ClC6H4, 4-MeC6H4, Me). The reaction of I or IV with Cl3CCN only gave the 1:1 products II or VI, resp. The 4,5-disubstituted imino-1,2,3,4-thiatriazoline VII reacted analogously to give the 4,5-disubstituted imino-1,2,4-thiadiazoline VIII.

IT 94295-69-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 94295-69-9 HCAPLUS

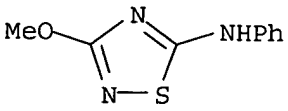
CN 1,2,4-Thiadiazol-5-amine, N-(4-chlorophenyl)-3-(2,2,2-trichloroethoxy)-(9CI) (CA INDEX NAME)



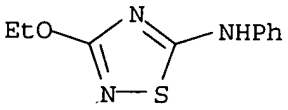
L10 ANSWER 11 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1962:473474 HCAPLUS
DOCUMENT NUMBER: 57:73474
ORIGINAL REFERENCE NO.: 57:14594a
TITLE: Thiadiazoles. XII. The ultraviolet absorption spectra of some 1,2,4-thiadiazoles
AUTHOR(S): Kurzer, Frederick; Taylor, Sheila A.
CORPORATE SOURCE: Univ. London
SOURCE: Journal of the Chemical Society (1962) 4191-200
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal

LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 57:73474
AB cf. CA 55, 17624h. The light-absorption properties, in the near-ultraviolet region, of several 1,2,4-thiadiazoles and their acyl derivs. are described, and are discussed with a view to establishing structural correlations. Spectra are also given of amidinothioureas, thiobiurets, and dithiobiurets, which yield the 1,2,4-thiadiazoles on oxidative cyclization.
IT 90564-94-6, 1,2,4-Thiadiazole, 5-anilino-3-methoxy-
90840-27-0, 1,2,4-Thiadiazole, 5-anilino-3-ethoxy-
(spectrum of)
RN 90564-94-6 HCAPLUS
CN 1,2,4-Thiadiazol-5-amine, 3-methoxy-N-phenyl- (9CI) (CA INDEX NAME)



RN 90840-27-0 HCAPLUS
CN 1,2,4-Thiadiazole, 5-anilino-3-ethoxy- (6CI, 7CI) (CA INDEX NAME)



L10 ANSWER 12 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1958:61148 HCAPLUS
DOCUMENT NUMBER: 52:61148
ORIGINAL REFERENCE NO.: 52:11016f-i,11017a-i,11018a-b
TITLE: Thiadiazoles. VI. 5-Amino-3-hydroxy-1,2,4-thiadiazole derivatives
AUTHOR(S): Kurzer, Frederick; Taylor, Sheila A.
CORPORATE SOURCE: Univ. London
SOURCE: Journal of the Chemical Society (1958) 379-86
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 52:61148
GI For diagram(s), see printed CA Issue.
AB cf. C.A. 51, 17895b. 1-Aryl(or alkyl)-2-thio-4-isobiurets (I), RNHCSNHC(OR'):NH, and the dealkylated 2-thiobiurets (II), RNHCSNHCONH2, were smoothly dehydrogenated by Br or H2O to 3-alkoxy(or hydroxy)-5-aryl(or alkyl)amino-1,2,4-thiadiazoles (III), RNHC:N.C(OR'):N.S. N-Aryl-N'-cyanoisothioureas (IV), RNHC(SNa):NCN, similarly afforded good yields of III (R' = H) (V). In the preparation of picrates, aqueous picric acid saturated at 30° was used. All I and II gave a precipitate of PbS when heated with Na plumbite [3N NaOH containing a few drops of 10% aqueous Pb(OAc)2] but IV resisted this reagent during 2 min. boiling. KOH (85%, 13.2 g.) in 50 ml. H2O treated successively with 22.1 g. H2NC(OMe):NH.HCl and 100 ml. Me2CO and the suspension stirred 30 min. with

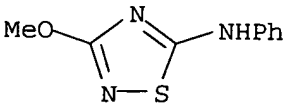
20-25 g. PhNCS under reflux, the Me2CO evaporated in vacuo, the residual two-phase system stirred into 300 g. crushed ice, and the solid product crystallized once from 170 ml. 15:2 C6H6-petr. ether and from C6H6 yielded 85% I (R = Ph, R' = Me) (VI), m. 129-31°. Condensation of 0.15 mole PhNCS and 0.225 mole H2NC(OEt):NH.HCl gave 23.4-26.7 g. I (R = Ph, R' = Et) (VII), m. 98-9°. VI (15.7 g.) in 150 ml. hot alc. refluxed 8-12 min. with 30 ml. concentrated HCl and the solution stirred into 1.2 l. H2O, the product kept 24 hrs. at 0°, and crystallized (2:1 alc.-petr. ether) gave 5.85-6.6 g. II (R = Ph) (VIII), m. 159-61°, also prepared by use of 2N alc. HCl (with persistent nauseating odor), and by hydrolysis of VII; picrate, m. 129-31° (alc.). VI (6.30 g.) in 75 ml. hot alc. cooled, the solution treated at 35-40° with 30 ml. freshly prepared ice-cold M Br in alc., the mixture poured into 750 ml. ice H2O, and the precipitate washed with H2O gave 75-85% III (R = Ph, R' = Me) (IX), m. 158-9° (10:3 Me2CO-EtOH), appreciably soluble in hot 3N aqueous NaOH, also obtained by treating 2.10 g. VI in 25 ml. boiling alc. with 1 ml. concentrated HCl and 5.7 ml. 6% H2O2 and 2 addnl. 5.7-ml. portions H2O2 at 3-min. intervals, stirring the pink turbid liquid into 150 ml. ice H2O and storing 12 hrs. at 0°, filtering, and crystallizing as above: mono-Ac derivative, m. 209-10° (Me2CO-EtOH); mono-Bz derivative, m. 180-1° (Me2CO-EtOH). Similarly, cyclizing VII with Br yielded 75-80% III (R = Ph, R' = Et) (X), m. 167-8° (alc.), also obtained in 80% yield by treating VII with H2O in the presence of mineral acid. Neither IX nor X gave a color with neutral FeCl3 solution VIII (5.85 g.) in 45 ml. alc. at 35-40° treated in 1 min. with 30 ml. M Br in CHCl3 (with external cooling) and the mixture added to 300 ml. H2O, the CHCl3 layer evaporated at room temperature and the residual solid added to the aqueous layer, filtered, and the product crystallized from Me2CO-EtOH and alc. gave V (R = Ph) (XI), m. 210-12°, also produced by treating 1.95 g. VIII in 20 ml. H2O containing 0.80 g. NaOH with 8.5 ml. 6% H2O 5 min. at 50° and filtering the cooled mixture, taking up the precipitate in 75 ml. hot H2O, and acidifying with dilute AcOH or HCl. Similarly, 1.99 g. IV (R = Ph) stirred at 45-50° in 5 ml. alc. and 3.3 ml. 3N NaOH and treated dropwise with 20 ml. 6% H2O2, the suspension kept 15 min. at 50° and diluted with 5 ml. alc., cooled to 0°, and filtered gave 42% XI. H2NCN (4.2 g.) in 6 ml. H2O successively treated with 10 ml. 10N NaOH, 6.75 g. PhNCS, and 10 ml. alc. and the single-phase mixture heated 18 min. on a steam bath, the yellow liquid diluted with 40 ml. H2O, treated at 30-40° with 6% H2O2 in 5-10 min. and kept 15 min. at 45°, the mixture cooled to 0°, and the separated Na salt acidified as above gave 5.40 g. XI; di-Bz derivative, m. 180-4°; di-Ac derivative, m. 253-5°; 3-p-tolylsulfonyloxy derivative, m. 160-2°. None of the derivs. gave a color reaction with neutral FeCl3 solution XI (3.86 g.) and 6 g. Zn turnings refluxed in 60 ml. alc. and treated dropwise in 8 min. with 5 ml. concentrated HCl, the refluxing continued 4 min. and the solution decanted, the residual Zn extracted 4 times with 5 ml. alc. and the alc. extract evaporated to 1/3 volume in vacuo, the concentrate stirred into ice H2O, and filtered gave 68% VIII, m. 157-9° (alc.). The filtrate contained no PhNH2. Similar reduction of IX gave 23% VIII and 15% PhNH2, identified as the Bz derivative Condensation of cyanamide with 7.45 g. p-MeC6H4NCS as above and collection of the Na salt at 0°, dissoln. in 150 ml. hot H2O containing a small amount of alkali, filtration, and acidification with concentrated HCl to Congo red with ice cooling gave 48% V (R = p-MeC6H4), m. 212-14° (1:1 Me2CO-EtOH). Na (3.22 g.) added during 8-12 min. to 125 ml. cold anhydrous

Me2CO and the suspension stirred at 35-40° with successive addition of 14.4 g. H2NC(OMe):NH.HCl and 8.0 g. MeNCS in 10 ml. Me2CO, the stirred suspension heated to boiling 5 min. and refluxed 30-45 min., the Me2CO evaporated in vacuo and the residue diluted with 75 ml. H2O, the aqueous layer extracted twice with 30 ml. Et2O and the exts. added to the organic layer, the mixture diluted with 100-150 ml. Et2O and washed 3 times with 10 ml. H2O, the extract dried (Na2SO4, 24 hrs.) and the filtered extract slowly treated with 28 ml. 3.5N HCl in alc., kept several hrs. at 0° and filtered, the precipitate washed with Et2O, and dried in vacuo yielded 65-72% I (R = R' = Me) (XII) HCl salt, m. 154-6°, giving a black precipitate with Na plumbite and yielding a low melting, amorphous XII; picrate, m. 154-6° (alc.). Similarly, interaction of Na, H2NC(OEt):NH.HCl, and MeNCS (with 15 min. refluxing) gave 60-70% crude HCl salt, m. 99-101°, crystallized from warm CHCl3 by dilution with Et2O to give I (R = Me, R' = Et) (XIII) HCl salt, m. 105-6° (decomposition); picrate, m. 125-6° (decomposition) (alc.). Crude XIII HCl salt from 0.11 mole MeNCS treated in 30 ml. H2O with 20 ml. 3N NaOH and the solid product washed with H2O, dried, and crystallized successively from C6H6 and dilute alc. yielded 62% XIII, m. 90-1°. XIII HCl salt (5.5 g.) boiled 12-15 min. in 60 ml. MeOH and 12 ml. concentrated HCl and the liquid evaporated in vacuo at 0° to 20 ml. and 5 ml. gave 3-3.5 g. product collected at both stages, purified by 3 crystns. from boiling H2O to yield 45-52% II (R = Me) (XIV), m. 174-5°. Similarly, hydrolysis of XIII in alc. in 18-20 min. yielded 68% XIV. Crude XII HCl salt (3.67 g.) in 10 ml. warm H2O treated with 20 ml. M Br in CHCl3 and the aqueous layer made alkaline with 3N NaOH, cooled to 0° and filtered, the filtrate evaporated, and the residue combined with the precipitate gave 58-68% product, crystallized successively from C6H6 and MeOH to give III (R = R' = Me), m. 120-1°; picrate, m. 155-7°. Oxidation of XIII HCl salt similarly yielded 80% of the corresponding III (R = Me, R' = Et), m. 122-3° (C6H6 and EtOH). XIV (1.0 g.) in 20 ml. MeOH treated with 7.5 ml. M Br in CHCl3 below 30° and the mixture kept 3 hrs. at 0°, filtered and the filtrate evaporated in vacuo, the residue and the precipitate combined and taken up in 4 ml. 3N NaOH, the solution made acid to litmus with 3N HCl, and filtered gave 0.37 g. V (R = Me), decomposing on heating and giving a purple color with FeCl3; picrate, m. 168-9° (decomposition) (1:1 H2O-EtOH); di-Bz derivative, m. 203-4° (decomposition) (Me2COEtOH).

IT 90564-94-6, 1,2,4-Thiadiazole, 5-anilino-3-methoxy-
90840-27-0, 1,2,4-Thiadiazole, 5-anilino-3-ethoxy-
(preparation of)

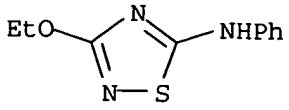
RN 90564-94-6 HCAPLUS

CN 1,2,4-Thiadiazol-5-amine, 3-methoxy-N-phenyl- (9CI) (CA INDEX NAME)

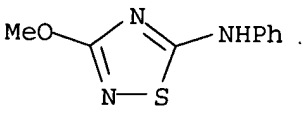


RN 90840-27-0 HCAPLUS

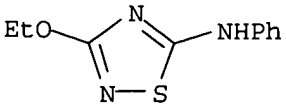
CN 1,2,4-Thiadiazole, 5-anilino-3-ethoxy- (6CI, 7CI) (CA INDEX NAME)



L10 ANSWER 13 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1957:43316 HCAPLUS
DOCUMENT NUMBER: 51:43316
ORIGINAL REFERENCE NO.: 51:8079a-b
TITLE: Cyclization of thiobiurets to substituted 1,2,4-thiadiazoles
AUTHOR(S): Kurzer, F.
CORPORATE SOURCE: Roy. Free Hosp. School Med., London
SOURCE: Chemistry & Industry (London, United Kingdom) (1956) 1482
CODEN: CHINAG; ISSN: 0009-3068
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB Dealkylation of PhNHCSNHC(OR):NH (I) gave PhNHCSNHCONH2 (II), m. 159-60°; dehydrogenation of I or II with Br or H2O2 gave good yields of S.N:C(OR).N:CNHPh (III). R and m.p. were given for I: Me, 129-30°; Et, 98-9°. For III: Me, 158-9°; Et, 167-8°; H, 212-13°.
IT 90564-94-6, 1,2,4-Thiadiazole, 5-anilino-3-methoxy-
90840-27-0, 1,2,4-Thiadiazole, 5-anilino-3-ethoxy-
(preparation of)
RN 90564-94-6 HCAPLUS
CN 1,2,4-Thiadiazol-5-amine, 3-methoxy-N-phenyl- (9CI) (CA INDEX NAME)



RN 90840-27-0 HCAPLUS
CN 1,2,4-Thiadiazole, 5-anilino-3-ethoxy- (6CI, 7CI) (CA INDEX NAME)



=> d l11 ibib abs hitstr tot

L11 ANSWER 1 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:900807 HCAPLUS
DOCUMENT NUMBER: 137:381259
TITLE: Preparation of 1,2,4-thiadiazole compounds and arthropodicides containing them

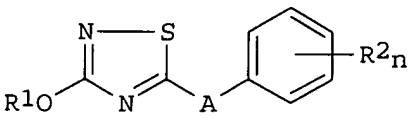
INVENTOR(S): Ihara, Hideki; Sakamoto, Noriyasu
PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.
CODEN: JKXXAF

DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002338557	A2	20021127	JP 2001-152269	20010522 <--
WO 2004041798	A1	20040521	WO 2002-JP11644	20021108
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002368330	A1	20040607	AU 2002-368330	20021108
BR 2002015911	A	20050726	BR 2002-15911	20021108
EP 1574505	A1	20050914	EP 2002-808100	20021108
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
CN 1688559	A	20051026	CN 2002-829792	20021108
US 2006167266	A1	20060727	US 2005-530136	20050404

PRIORITY APPLN. INFO.: JP 2001-152269 A 20010522
WO 2002-JP11644 A 20021108

OTHER SOURCE(S): MARPAT 137:381259
GI



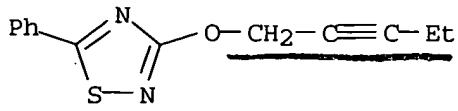
I

AB The compds. I [R1 = C3-7 (halo)alkenyl; R2 = halo, C1-4 alkyl, C1-3 haloalkyl, C1-4 haloalkoxy, cyano, NO2; n = 0-5; A = O, S,direct bond, CR3R4, NR5; R3, R4 = H, C1-4 alkyl; R5 = H, C1-7 alkyl, C1-3 haloalkyl, C2-4 (halo)alkoxyalkyl, C3-6 (halo)alkenyl, C3-7 (halo)alkynyl, CH2CN] and arthropod control agents containing I are claimed. A composition containing 5-phenyl-3-propargyloxy-1,2,4-thiadiazole (preparation given), showed ≥90% control against Aphis gossypii parasitic on cucumber seedlings.

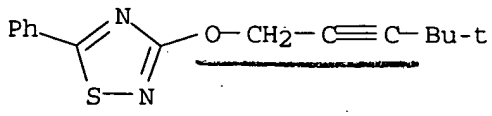
IT 476315-98-7 476315-99-8 476316-00-4
476316-01-5 476316-02-6 476316-03-7
476316-04-8 476316-05-9 476316-06-0
476316-07-1 476316-08-2 476316-09-3
476316-10-6 476316-11-7 476316-12-8
476316-13-9 476316-68-4 476316-72-0
476316-74-2
RL: AGR (Agricultural use); BSU (Biological study, unclassified); BIOL

(Biological study); USES (Uses)
(preparation of 1,2,4-thiadiazole compds. as arthropodicides)

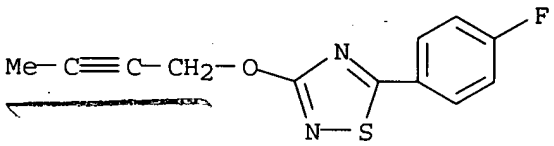
RN 476315-98-7 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-pentynyloxy)-5-phenyl- (9CI) (CA INDEX NAME)



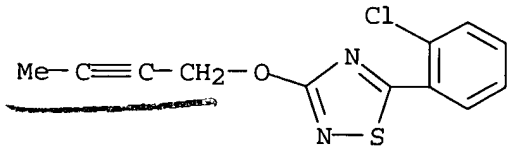
RN 476315-99-8 HCAPLUS
CN 1,2,4-Thiadiazole, 3-[(4,4-dimethyl-2-pentynyl)oxy]-5-phenyl- (9CI) (CA INDEX NAME)



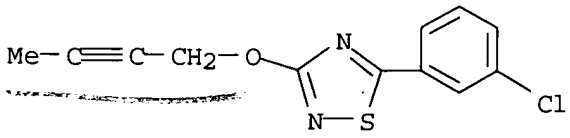
RN 476316-00-4 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(4-fluorophenyl)- (9CI) (CA INDEX NAME)



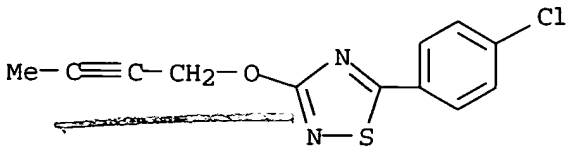
RN 476316-01-5 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(2-chlorophenyl)- (9CI) (CA INDEX NAME)



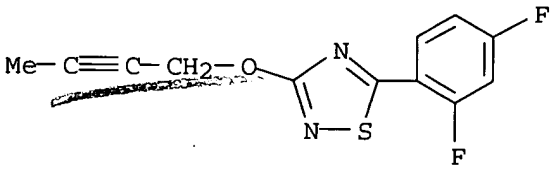
RN 476316-02-6 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(3-chlorophenyl)- (9CI) (CA INDEX NAME)



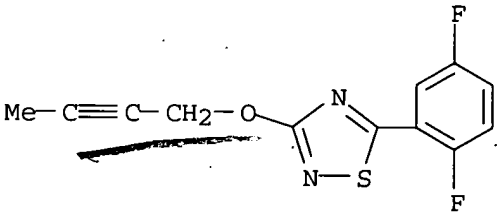
RN 476316-03-7 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(4-chlorophenyl)- (9CI) (CA INDEX NAME)



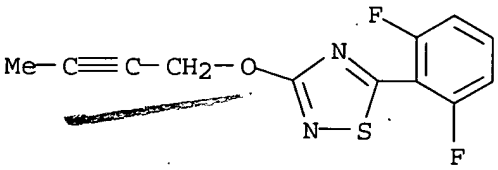
RN 476316-04-8 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(2,4-difluorophenyl)- (9CI) (CA INDEX NAME)



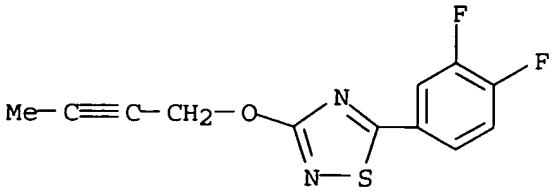
RN 476316-05-9 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(2,5-difluorophenyl)- (9CI) (CA INDEX NAME)



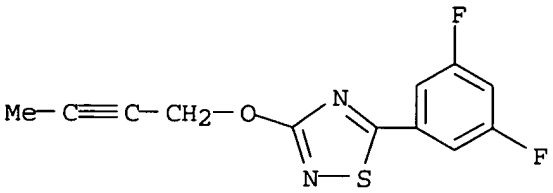
RN 476316-06-0 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(2,6-difluorophenyl)- (9CI) (CA INDEX NAME)



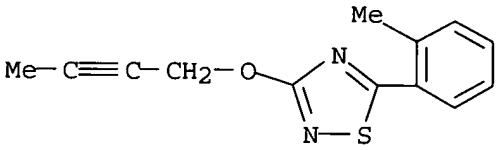
RN 476316-07-1 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(3,4-difluorophenyl)- (9CI) (CA INDEX NAME)



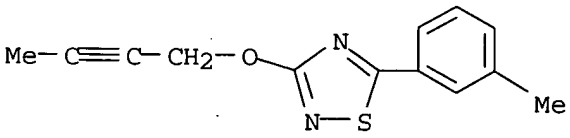
RN 476316-08-2 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(3,5-difluorophenyl)- (9CI) (CA INDEX NAME)



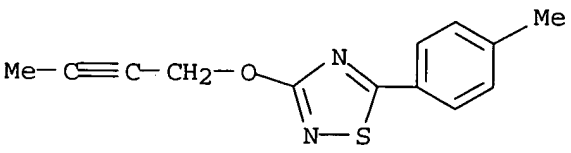
RN 476316-09-3 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(2-methylphenyl)- (9CI) (CA INDEX NAME)



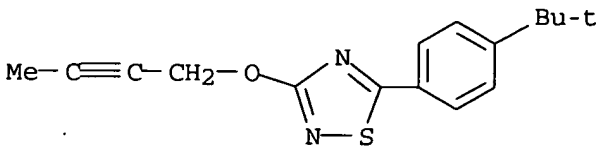
RN 476316-10-6 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(3-methylphenyl)- (9CI) (CA INDEX NAME)



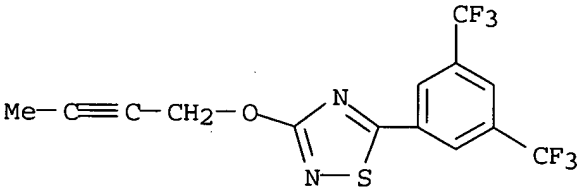
RN 476316-11-7 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(4-methylphenyl)- (9CI) (CA INDEX NAME)



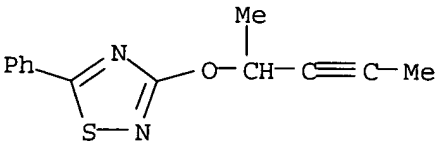
RN 476316-12-8 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-[4-(1,1-dimethylethyl)phenyl]- (9CI) (CA INDEX NAME)



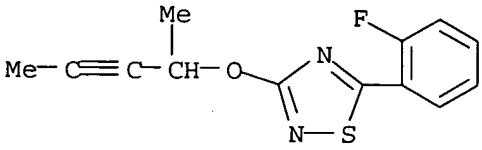
RN 476316-13-9 HCAPLUS
CN 1,2,4-Thiadiazole, 5-[3,5-bis(trifluoromethyl)phenyl]-3-(2-butynyloxy)- (9CI) (CA INDEX NAME)



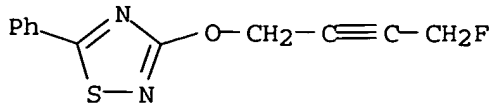
RN 476316-68-4 HCAPLUS
CN 1,2,4-Thiadiazole, 3-[(1-methyl-2-butynyl)oxy]-5-phenyl- (9CI) (CA INDEX NAME)



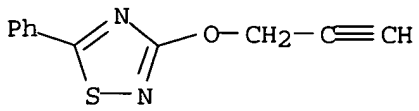
RN 476316-72-0 HCAPLUS
CN 1,2,4-Thiadiazole, 5-(2-fluorophenyl)-3-[(1-methyl-2-butynyl)oxy]- (9CI) (CA INDEX NAME)



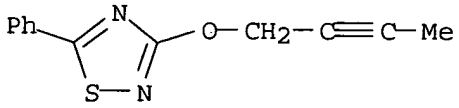
RN 476316-74-2 HCAPLUS
CN 1,2,4-Thiadiazole, 3-[(4-fluoro-2-butynyl)oxy]-5-phenyl- (9CI) (CA INDEX NAME)



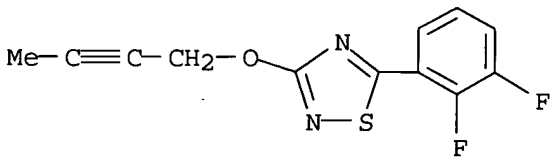
IT 476315-86-3P 476315-87-4P 476315-89-6P
476315-92-1P 476315-94-3P
RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 1,2,4-thiadiazole compds. as arthropodicides)
RN 476315-86-3 HCAPLUS
CN 1,2,4-Thiadiazole, 5-phenyl-3-(2-propynyloxy)- (9CI) (CA INDEX NAME)



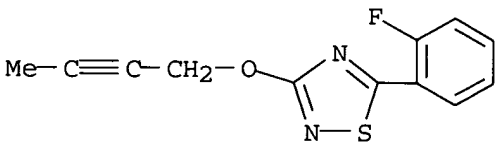
RN 476315-87-4 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-phenyl- (9CI) (CA INDEX NAME)



RN 476315-89-6 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(2,3-difluorophenyl)- (9CI) (CA INDEX NAME)

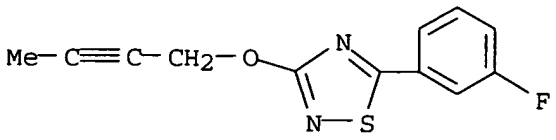


RN 476315-92-1 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(2-fluorophenyl)- (9CI) (CA INDEX NAME)



RN 476315-94-3 HCAPLUS

CN 1,2,4-Thiadiazole, 3-(2-butynyloxy)-5-(3-fluorophenyl)- (9CI) (CA INDEX NAME)

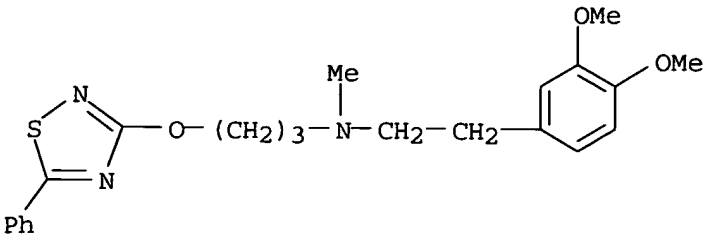


L11 ANSWER 2 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:738242 HCAPLUS
DOCUMENT NUMBER: 138:280905
TITLE: Anti-ischemic Compound KC 12291 Prevents Diastolic Contracture in Isolated Atria by Blockade of Voltage-Gated Sodium Channels
AUTHOR(S): Tamareille, Sophie; Le Grand, Bruno; John, Gareth W.; Feuvray, Danielle; Coulombe, Alain
CORPORATE SOURCE: Hospital Marie Lannelongue, Universite Paris Sud XI, paris, Fr.
SOURCE: Journal of Cardiovascular Pharmacology (2002), 40(3), 346-355
CODEN: JCPCDT; ISSN: 0160-2446
PUBLISHER: Lippincott Williams & Wilkins
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Several lines of evidence support a fundamental role for voltage-gated sodium channels in mediating ischemic Na rise. We examined the effect of the novel anti-ischemic compound KC 12291 on veratridine-stimulated and lysophosphatidylcholine (LPC)-induced sustained sodium current (INaL) mediated by sodium channels in isolated myocytes obtained from guinea-pig atria, by using the whole-cell patch-clamp technique. We also analyzed the effect of KC 12291 on veratridine- and LPC-induced contractures in isolated guinea-pig atria. Veratridine as well as LPC increased INaL measured at 20 ms of a 2 s pulse evoked from -100 to -30 mV (47.5 and 12 pA/pF in the presence of 40 μ veratridine and 10 μ LPC, resp., vs. 6.7 pA/pF under control conditions). A significant reduction by KC 12291 in the quantity of charge carried by veratridine-stimulated INaL in the range of test potentials between -50 mV and +10 mV was observed and similar effects were obtained on LPC-induced INaL. Thus, the quantity of charge carried by LPC-induced INaL over a 2 s pulse to -30 mV was reduced by 48% in the presence of 10 μ KC 12291 vs. a reduction by 50% of veratridine-stimulated INaL at the same test potential. Veratridine- and LPC-induced submaximal contractures in isolated atria were significantly inhibited by KC 12291 in a concentration-dependent manner, with an IC of 0.55 μ and 0.79 μ, resp. The data indicate that veratridine- and LPC-induced increases in diastolic tension are inhibited by KC 12291 by a mechanism that involves blockade of voltage-gated sodium channels mediating sustained sodium current.

IT 181936-98-1, KC 12291
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(KC 12291 inhibits voltage-gated sodium channels and prevents diastolic contracture in atrial myocytes)

RN 181936-98-1 HCAPLUS
CN Benzeneethanamine, 3,4-dimethoxy-N-methyl-N-[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)



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REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

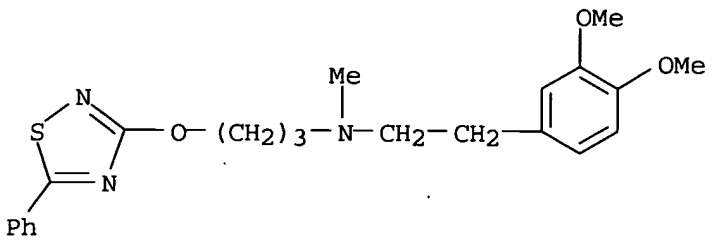
L11 ANSWER 3 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:908531 HCAPLUS
DOCUMENT NUMBER: 134:351537
TITLE: Multinuclear MR-spectroscopy on ion-homeostasis and energetics during ischemia and reperfusion
AUTHOR(S): Decking, Ulrich K. M.; Vogler, Lars; Hartmann, Matthias; Schrader, Jurgen
CORPORATE SOURCE: Department of Physiology, Heinrich-Heine-University, Dusseldorf, 40001, Germany
SOURCE: Magnetic Resonance Materials in Physics, Biology and Medicine (2000), 11(1-2), 3-4
CODEN: MRBMEQ; ISSN: 1352-8661
PUBLISHER: Elsevier Science Ireland Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB To develop a coherent model of ion homeostasis in the course of ischemia, intracellular Na+, pH and energy status as well as cardiac contractile functions were measured in the saline perfused guinea pig heart. To sensitively detect small changes of Na+ upon the start of ischemia, triple quantum filtered 23Na NMR spectra were acquired in the presence of shift reagent. Intracellular pH and energy status were assessed by 31P NMR. The effects of Na+-H+-exchanger (NHE) inhibition were further evaluated in both stop-flow and low flow ischemia. Results showed that Na+-channels constitute a major part of Na+ entry in the initial minutes following the onset of ischemia. The persistent component of the Na+ current does not play a significant role in the guinea pig heart even thereafter. Due to intracellular acidification, NHE is activated and forms the dominant influx pathway in the next 30 min of ischemia, but is partially inactivated in the later course of ischemia. Alternative, not yet characterized ports of entry gain importance in this phase. Blocking either voltage-gated Na+-channels or NHE improved post-ischemic contractile function. Thus, reducing Na+ overload in ischemia is a promising therapeutic approach for cardioprotection.

IT 181936-98-1, KC 12291
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(multinuclear MR-spectroscopy on ion-homeostasis and energetics during ischemia and reperfusion)

RN 181936-98-1 HCAPLUS
CN Benzeneethanamine, 3,4-dimethoxy-N-methyl-N-[3-[(5-phenyl-1,2,4-thiadiazol-

3-yl)oxy]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)



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REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 4 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:97883 HCAPLUS
DOCUMENT NUMBER: 132:273796
TITLE: Primary porcine enterocyte and hepatocyte cultures to study drug oxidation reactions
AUTHOR(S): Bader, A.; Hansen, T.; Kirchner, G.; Allmeling, C.; Haverich, A.; Borlak, J. T.
CORPORATE SOURCE: Leibniz Research Laboratories for Biotechnology and Artificial Organs, Leibniz Research Laboratories for Biotechnology and Artificial Organs, Forschungszentrum der MHH, Hannover, D-30659, Germany
SOURCE: British Journal of Pharmacology (2000), 129(2), 331-342
CODEN: BJPCBM; ISSN: 0007-1188
PUBLISHER: Nature Publishing Group
DOCUMENT TYPE: Journal
LANGUAGE: English

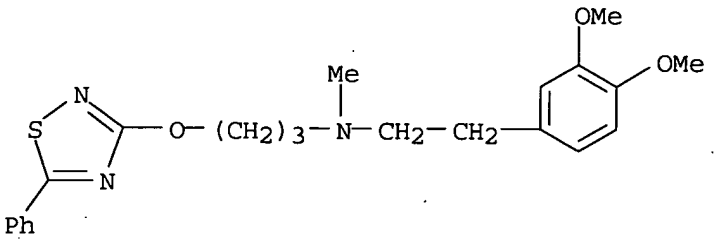
AB Primary porcine hepatocytes and enterocytes were isolated and cultured in Williams' E medium for up to 10 days to investigate potential organ differences in the metabolism of the immunosuppressive compound tacrolimus (FK 506) and of two investigational drugs (KC11346 and KC12291). Using LC-MS (FK506) and HPLC-FL (KC 11346/12291) a number of metabolites with identical mass and/or identical retention time could be detected. In the case of tacrolimus hepatocytes and enterocytes produced the same spectrum of metabolites, e.g. bisdemethyl-tacrolimus, demethyl-tacrolimus, demethyl-hydroxy-tacrolimus and hydroxy-tacrolimus, albeit at varying intensities. Treatment of enterocyte cultures with dexamethasone increased the overall metabolite formation very significantly (up to 36 fold). The metabolism of tacrolimus was also studied with prepns. of insect cells, that express specifically high levels of individual human cytochrome P 450 (CYP) isoenzymes. All metabolites could be generated with microsomal prepns. specifically expressing CYP3A4, but hydroxytacrolimus was exclusively produced by CYP3A5. In the case of the investigational drugs KC 11346 and KC 12291 only three metabolites were formed by cultured enterocytes whereas hepatocytes produced 10 and 20 metabolites, resp. When assessed at the protein level CYP1A and CYP3A were expressed in cultures of porcine enterocytes for up to 10 days but porcine hepatocytes expressed addnl. CYP2C9/10. In conclusion, primary enterocytes and hepatocytes can be successfully cultured for several days

while maintaining mono-oxygenase activity and may therefore be used as a tool for studying intestinal and hepatic metabolism

IT 181936-98-1, KC12291
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(biotransformation of tacrolimus and other drugs in primary porcine enterocyte vs. hepatocyte cultures)

RN 181936-98-1 HCAPLUS

CN Benzeneethanamine, 3,4-dimethoxy-N-methyl-N-[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)



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REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 5 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:691080 HCAPLUS

DOCUMENT NUMBER: 130:148417

TITLE: Cardioprotective actions of KC 12291. II. Delaying Na+ overload in ischemia improves cardiac function and energy status in reperfusion

AUTHOR(S): Hartmann, Matthias; Decking, U. K. M.; Schrader, Jurgen

CORPORATE SOURCE: Institut fur Herz- und Kreislaufphysiologie, Heinrich-Heine-Universitat Dusseldorf, Postfach 10 10 07, Dusseldorf, D-40001, Germany

SOURCE: Naunyn-Schmiedeberg's Archives of Pharmacology (1998), 358(5), 554-560
CODEN: NSAPCC; ISSN: 0028-1298

PUBLISHER: Springer-Verlag

DOCUMENT TYPE: Journal

LANGUAGE: English

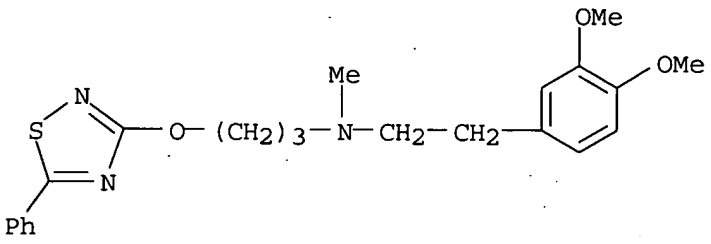
AB The novel blocker of voltage-gated Na+ channels KC 12291 (1-(5-phenyl-1,2,4-thiadiazol-3-yl-oxypropyl)-3-[N-methyl-N-[2-(3,4-dimethoxyphenyl)ethyl] amino] propane hydrochloride) delays myocardial Na+ overload in ischemia. To test whether KC 12291 displays cardioprotective properties in the intact heart, cardiac function, energy status and intracellular pH (31P NMR) as well as ion homeostasis (23Na NMR) were investigated during low-flow ischemia (100 μl/min for 36 min) followed by reperfusion. In the well-oxygenated, isolated perfused guinea pig heart, KC 12291 (1 μM) had no effect on left ventricular developed pressure (LVDP; 54±19 mmHg). KC 12291 delayed the onset and decreased the extent of ischemic contracture and markedly improved the recovery of LVDP in reperfusion [39±14 mmHg (n=4) vs 2±2 mmHg in controls (n=5)]. KC 12291 did not influence the rapid drop in phosphocreatine

(PCr) following onset of ischemia but attenuated the decline in ATP. It also diminished the ischemia-induced fall in intracellular pH [6.39±0.2 (n=6) vs 6.18±0.20 in controls (n=6)]. In reperfusion, KC 12291 remarkably enhanced the recovery of PCr (84.8±9.6% vs 51.1±8.8% of baseline) and ATP (38.2±12.9% vs 23.7±9.3% of baseline). It also accelerated the recovery of intracellular pH. KC 12291 not only reduced the extent of ischemia-induced Na+ overload, but also enhanced Na+ recovery. It is concluded that KC 12291 delays contracture and reduces ATP depletion and acidosis in ischemia, and markedly improves the functional, energetic and ionic recovery in reperfusion. Blocking voltage-gated Na+ channels in ischemia to delay Na+ overload may thus constitute a promising therapeutic approach for cardioprotection.

IT 181936-98-1, KC 12291
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(cardioprotective actions of KC 12291: delaying Na+ overload in ischemia improves cardiac function and energy status in reperfusion)

RN 181936-98-1 HCAPLUS

CN Benzeneethanamine, 3,4-dimethoxy-N-methyl-N-[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)



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REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 6 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:691078 HCAPLUS

DOCUMENT NUMBER: 130:162913

TITLE: Cardioprotective actions of KC 12291 I. Inhibition of voltage-gated Na+ channels in ischemia delays myocardial Na+ overload

AUTHOR(S): Decking, U. K. M.; Hartmann, Matthias; Rose, Horst; Bruckner, Reinhard; Meil, Jorg; Schrader, Jurgen

CORPORATE SOURCE: Institut fur Herz- und Kreislaufphysiologie, Heinrich-Heine-Universitat Dusseldorf, Postfach 10 10 07, Dusseldorf, D-40001, Germany

SOURCE: Naunyn-Schmiedeberg's Archives of Pharmacology (1998), 358(5), 547-553
CODEN: NSAPCC; ISSN: 0028-1298

PUBLISHER: Springer-Verlag

DOCUMENT TYPE: Journal

LANGUAGE: English

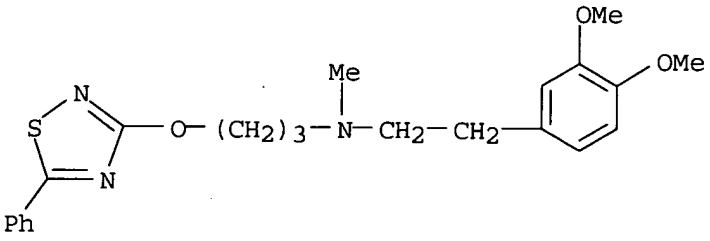
AB To characterize KC 12291 (1-(5-phenyl-1,2,4-thiadiazol-3-yl-oxypropy)-3-[N-methyl-[2-(3,4-dime-thoxyphenyl) ethyl] amino] propane hydrochloride), a

newly synthesized inhibitor of voltage-gated Na+ channels, the effects of the agent on Na+ current and ischemia-induced Na+ overload were investigated in isolated cardiomyocytes, atria and saline-perfused hearts. As measured by the patch clamp technique, KC 12291 (1 μM) significantly reduced peak Na+ current after activation of voltage-gated Na+ channels in rat cardiomyocytes. Partial depolarization enhanced the inhibitory effects during steady state conditions of the channel. In isolated guinea pig atria, 1 μM KC 12291 had no effect on contractility under basal conditions but effectively delayed the onset and reduced the extent of anoxic contracture. The concentration-response curve was clearly shifted to the left when atria were partially depolarized by increased extracellular K+. As measured by 23Na NMR spectroscopy in isolated perfused guinea pig hearts, intracellular Na+ rose more than four-fold in a linear fashion during 60 min of low-flow ischemia. KC 12291 (1 μM) prevented Na+ overload within the initial 12 min of ischemia; thereafter the slope of Na+ accumulation was identical to controls. Elec. excitability of hearts, evaluated by intracardial ECG, completely ceased within 15 min after the onset of ischemia. KC 12291 (1 μM) accelerated this process by more than 6 min. The data provide first evidence that KC 12291 reduces Na+ influx through voltage-gated Na+ channels during ischemia and thus delays Na+ overload by enhancing the inexcitability of the heart.

IT 181936-98-1, KC 12291
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(cardioprotective actions of KC 12291: inhibition of voltage-gated sodium channels in ischemia delays myocardial sodium overload)

RN 181936-98-1 HCAPLUS

CN Benzeneethanamine, 3,4-dimethoxy-N-methyl-N-[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)



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REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

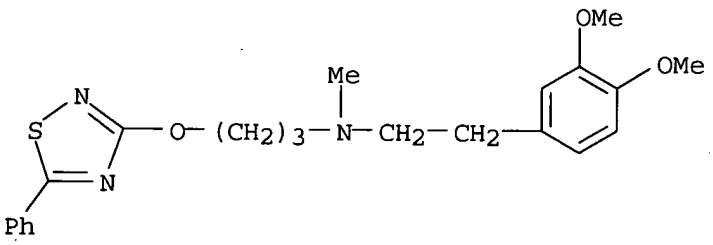
L11 ANSWER 7 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:55258 HCAPLUS
DOCUMENT NUMBER: 128:212570
TITLE: Sensitive method for the determination of KC 12291 in rat plasma and urine by high-performance liquid chromatography
AUTHOR(S): Tomori, E.; Tormasi, E.; Varga, M.; Borlak, J.
CORPORATE SOURCE: Institute for Drug Research Ltd., P.O. Box 82, Budapest, H-1325, Hung.

SOURCE: Journal of Chromatography, B: Biomedical Sciences and Applications (1998), 705(1), 105-110
CODEN: JCBBEP; ISSN: 0378-4347
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A sensitive and selective ion-pair reversed-phase HPLC method has been developed for the quant. determination of KC 12291 and its major metabolite, KC 13194, in rat plasma and urine. An Ultrasphere ODS column constructed by using a mobile phase of 1 mM 1-octanesulfonic acid containing acetonitrile-0.1 M triethylamine phosphate buffer, pH 2.2 (29:71, volume/volume in plasma and 27:73, volume/volume in urine), an internal standard and a fluorescent detector (excitation 265 nm, emission 370 nm) were used for the separation and the quant. determination, resp. The plasma samples were made alkaline and both compds.
were cleaned up by the use of liquid-liquid extraction The limit of quantification
was 10 ng/mL for KC 12291 in plasma and urine and for KC 13194 and 100 ng/mL in plasma, resp. The assay has been validated with respect to system suitability, accuracy, precision, recovery, stability and ruggedness. All validated parameters were found to be within the necessary limits.

IT 181936-98-1, KC 12291 181938-50-1, KC 13194
RL: ANT (Analyte); ANST (Analytical study)
(KC 12291 and its metabolite KC 13194 determination in plasma and urine by HPLC)

RN 181936-98-1 HCAPLUS
CN Benzeneethanamine, 3,4-dimethoxy-N-methyl-N-[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)



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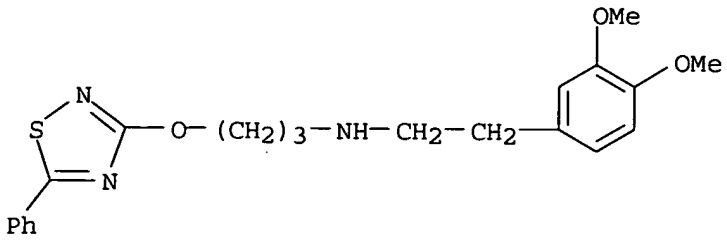
RN 181938-50-1 HCAPLUS
CN Benzeneethanamine, 3,4-dimethoxy-N-[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)



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REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 8 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:537795 HCAPLUS
DOCUMENT NUMBER: 125:247807
TITLE: (Phenylalkylaminoalkyloxy)-heteroaryl compounds having heart-rate-lowering and anti-ischemic effects
INVENTOR(S): Kehrbach, Wolfgang; Mlinaric, Michael; Ziegler, Dieter; Brueckner, Reinhard; Bielenberg, Willi
PATENT ASSIGNEE(S): Kali-Chemie Pharma GmbH, Germany
SOURCE: U.S., 34 pp., Cont.-in-part of U.S. Ser. No. 352, 353, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5547967	A	19960820	US 1995-476118	19950607 <--
DE 4341749	A1	19950614	DE 1993-4341749	19931208 <--
DE 19513503	A1	19961017	DE 1995-19513503	19950410 <--
US 5679699	A	19971021	US 1995-576699	19951221 <--
EP 737680	A1	19961016	EP 1996-105335	19960403 <--
EP 737680	B1	20040303		
R: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
AT 260905	E	20040315	AT 1996-105335	19960403
ES 2213165	T3	20040816	ES 1996-105335	19960403
JP 09151180	A2	19970610	JP 1996-88590	19960410 <--

PRIORITY APPLN. INFO.:

DE 1993-4341749	A	19931208
US 1994-352353	B2	19941208
DE 1995-19513503	A	19950410
US 1995-476118	A3	19950607

OTHER SOURCE(S): MARPAT 125:247807
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB 3-(Phenylalkylaminoalkyloxy)heteroaryl compds. having heart rate lowering

and/or anti-ischemic effects, methods for their preparation and pharmaceutical compns. containing them are described. The compds. correspond to the general formula I in which n is an integer from 1-5, A = NR1Q in which R1 represents hydrogen or a lower alkyl group and Q represents a (CH2)m group in which m is 2 to 8 and which may optionally be substituted in the α position to the oxygen atom by 1 or 2 lower alkyl groups, or Q represents a 2-hydroxypropylene chain, or A = [cyclic N(CH2)p]-B in which p is 4 to 6 and B represents a (CH2)r group in which r is 1 to 3 and which may optionally be substituted in the α position to the oxygen atom by 1 or 2 lower alkyl groups; R2 = e.g., H, halogen, lower alkyl; R3 = e.g., H, halogen, lower alkyl; R4 = H or lower alkyl; R5 is disposed in the 1 or 2 position and represents hydrogen, lower alkyl or a phenyl-lower alkyl group; R6 = e.g., H, lower alkyl, lower alkoxy; R7 = e.g., H, lower alkyl, lower alkoxy, and their acid addition salts. The compds. also correspond to the general formula II wherein R1 = H or lower alkyl; R2 = e.g., H, halo, lower alkyl; R3 = e.g., H, halo, lower alkyl; R4 = thienyl or R5R6-substituted Ph wherein R5 = e.g., H, halo, lower alkyl and R6 = e.g., H, halo, lower alkyl; A = N or R7C in which R7 = H or lower alkyl; B = O or, if A = N, also S; n = an integer from 1-5; and Q = (CH2)m where m is an integer from 2-8 and which may optionally be substituted by a lower alkyl, or represents the 2-hydroxypropylene chain, or a physiol. acceptable acid addition salt thereof. Thus, e.g., alkylation of 5-(3,4-dimethoxyphenyl)pyrazolin-3-one (preparation given) with 3-[N-(2-(3,4-dimethoxyphenyl)ethyl)-N-methylamino]propyl chloride (preparation given) afforded aminoalkoxypyrazole III which exhibited FRQ 75 (that concentration, in μmol/L, at which 20 min after the administration of the substance there is a reduction in the heart rate to 75% of the initial value) = = 1.6. Data were also presented for cytoprotective effect on atrial contraction induced by hypoxia (as low as 0.55 μM), and for corresponding force recovery after hypoxia (up to 80%). Pharmaceutical formulations were given.

IT 181935-23-9P 181935-25-1P 181935-26-2P
181935-28-4P 181935-29-5P 181935-31-9P
181935-32-0P 181935-37-5P 181936-98-1P
181937-06-4P 181937-10-0P 181937-18-8P
181937-24-6P 181937-26-8P 181937-28-0P
181937-36-0P 181937-41-7P 181937-74-6P
181938-14-7P 181938-16-9P 181938-19-2P
181938-22-7P 181938-25-0P 181938-28-3P
181938-34-1P 181938-39-6P 181938-41-0P
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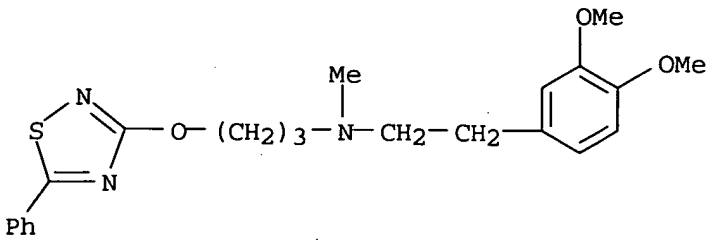
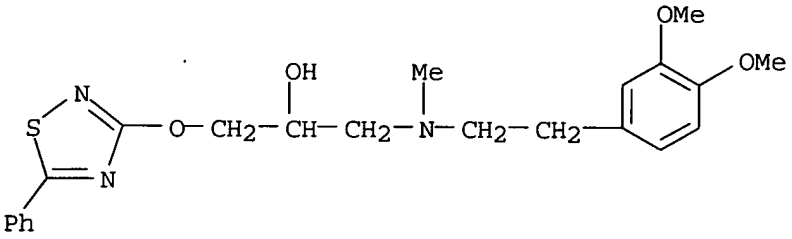
181938-57-8P 181938-59-0P 181938-60-3P
181938-61-4P 181938-64-7P 181938-66-9P
181938-71-6P 181938-73-8P 181938-75-0P
181954-84-7P 181954-88-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
((phenylalkylaminoalkyloxy)-heteroaryl compds. having heart-rate-lowering and anti-ischemic effects)

RN 181935-23-9 HCAPLUS

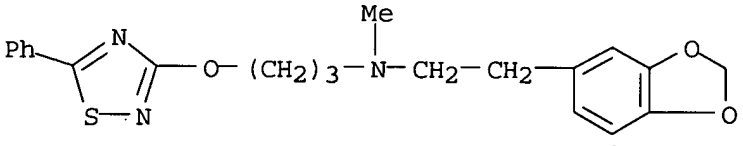
CN Benzeneethanamine, 3,4-dimethoxy-N-methyl-N-[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]- (9CI) (CA INDEX NAME)



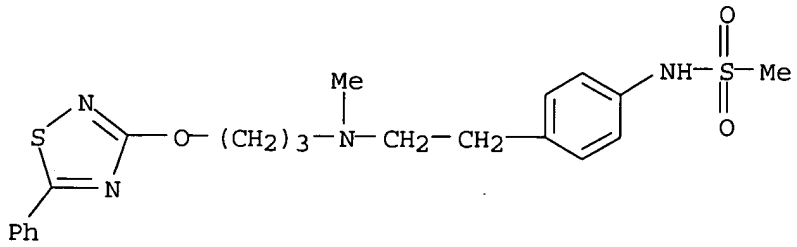
RN 181935-25-1 HCAPLUS
CN 2-Propanol, 1-[[2-(3,4-dimethoxyphenyl)ethyl]methylamino]-3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]- (9CI) (CA INDEX NAME)



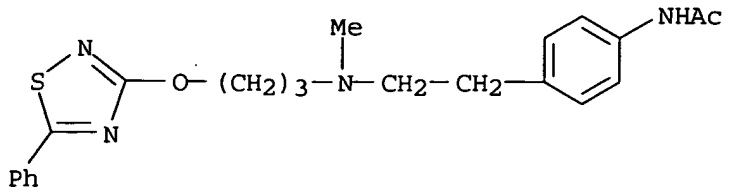
RN 181935-26-2 HCAPLUS
CN 1,3-Benzodioxole-5-ethanamine, N-methyl-N-[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]- (9CI) (CA INDEX NAME)



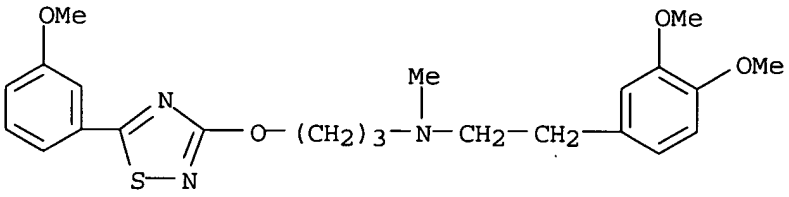
RN 181935-28-4 HCAPLUS
CN Methanesulfonamide, N-[4-[2-[methyl[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]amino]ethyl]phenyl]- (9CI) (CA INDEX NAME)



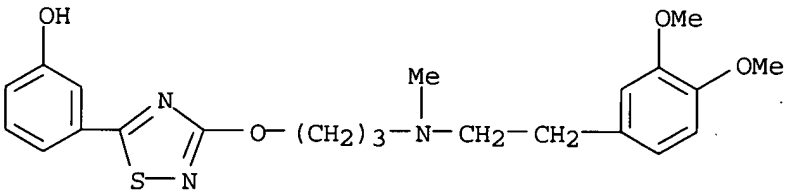
RN 181935-29-5 HCAPLUS
CN Acetamide, N-[4-[2-[methyl[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]amino]ethyl]phenyl]- (9CI) (CA INDEX NAME)



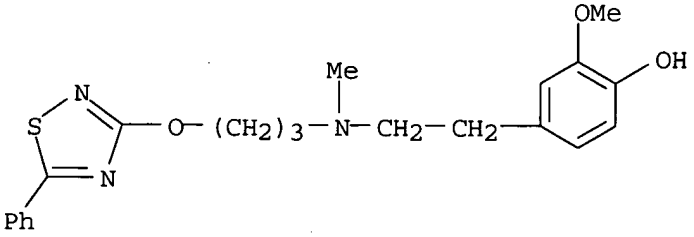
RN 181935-31-9 HCAPLUS
CN Benzeneethanamine, 3,4-dimethoxy-N-[3-[[5-(3-methoxyphenyl)-1,2,4-thiadiazol-3-yl]oxy]propyl]-N-methyl- (9CI) (CA INDEX NAME)



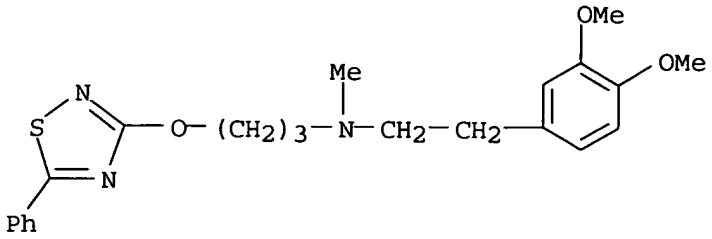
RN 181935-32-0 HCAPLUS
CN Phenol, 3-[3-[3-[[2-(3,4-dimethoxyphenyl)ethyl]methylamino]propoxy]-1,2,4-thiadiazol-5-yl]- (9CI) (CA INDEX NAME)



RN 181935-37-5 HCAPLUS
CN Phenol, 2-methoxy-4-[2-[methyl[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]amino]ethyl]- (9CI) (CA INDEX NAME)

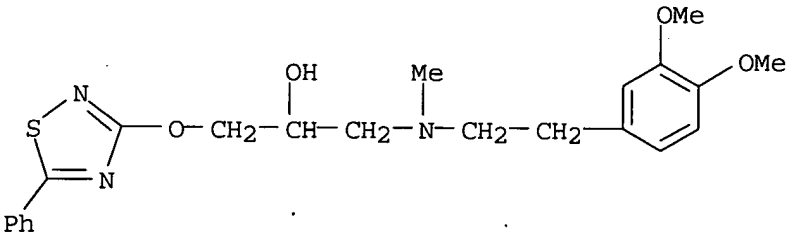


RN 181936-98-1 HCAPLUS
CN Benzeneethanamine, 3,4-dimethoxy-N-methyl-N-[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)



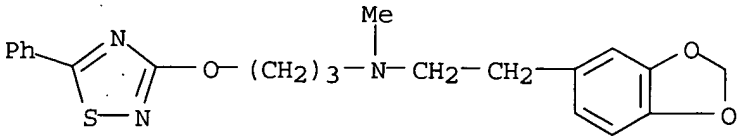
● HCl

RN 181937-06-4 HCAPLUS
CN 2-Propanol, 1-[[2-(3,4-dimethoxyphenyl)ethyl]methylamino]-3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]-, monohydrochloride (9CI) (CA INDEX NAME)



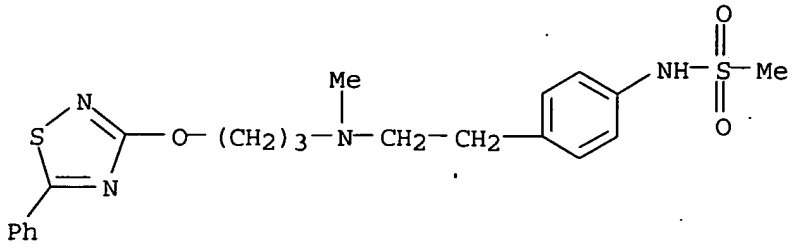
● HCl

RN 181937-10-0 HCAPLUS
CN 1,3-Benzodioxole-5-ethanamine, N-methyl-N-[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)



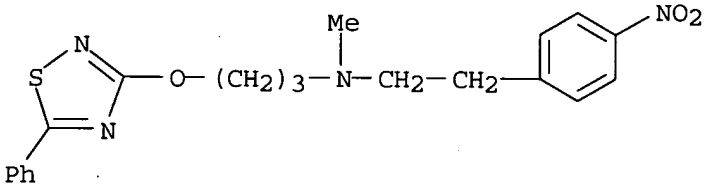
● HCl

RN 181937-18-8 HCAPLUS
CN Methanesulfonamide, N-[4-[2-[methyl[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]amino]ethyl]phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)



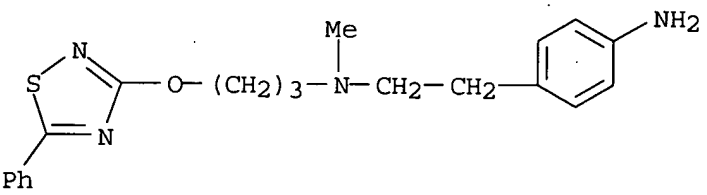
● HCl

RN 181937-24-6 HCAPLUS
CN Benzeneethanamine, N-methyl-4-nitro-N-[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)



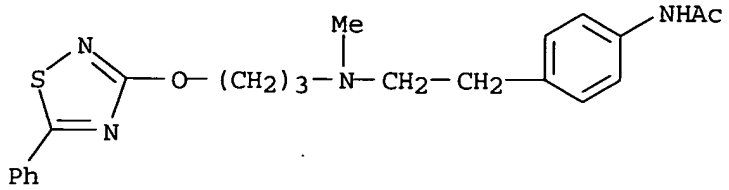
● HCl

RN 181937-26-8 HCAPLUS
CN Benzeneethanamine, 4-amino-N-methyl-N-[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)



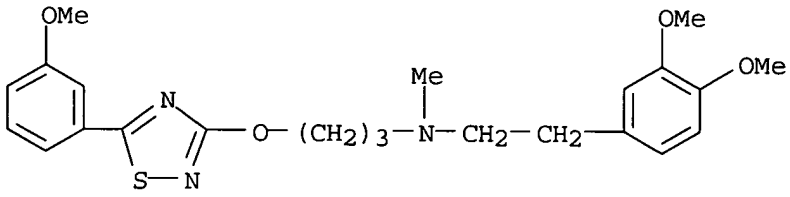
● HCl

RN 181937-28-0 HCAPLUS
CN Acetamide, N-[4-[2-[methyl[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]amino]ethyl]phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)



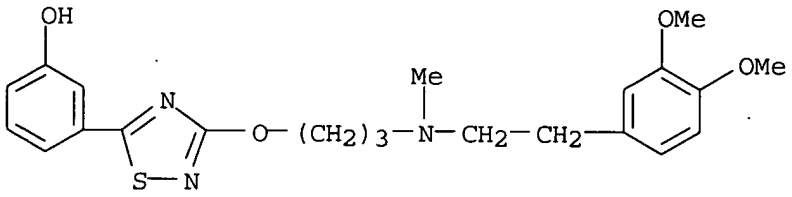
● HCl

RN 181937-36-0 HCAPLUS
CN Benzeneethanamine, 3,4-dimethoxy-N-[3-[[5-(3-methoxyphenyl)-1,2,4-thiadiazol-3-yl]oxy]propyl]-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



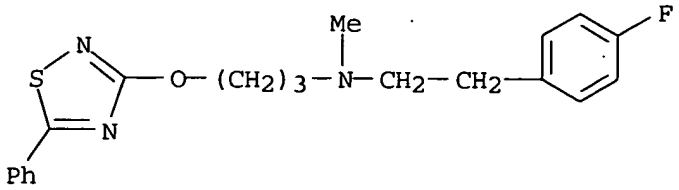
● HCl

RN 181937-41-7 HCAPLUS
CN Phenol, 3-[3-[3-[[2-(3,4-dimethoxyphenyl)ethyl]methylamino]propoxy]-1,2,4-thiadiazol-5-yl]-, monohydrochloride (9CI) (CA INDEX NAME)



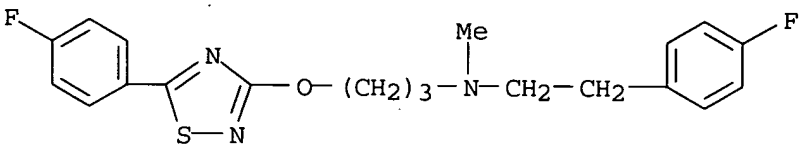
● HCl

RN 181937-74-6 HCAPLUS
CN Benzeneethanamine, 4-fluoro-N-methyl-N-[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)



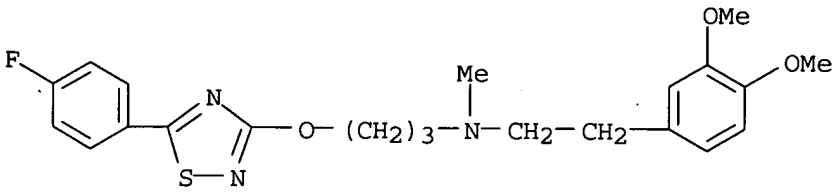
● HCl

RN 181938-14-7 HCAPLUS
CN Benzeneethanamine, 4-fluoro-N-[3-[[5-(4-fluorophenyl)-1,2,4-thiadiazol-3-yl]oxy]propyl]-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



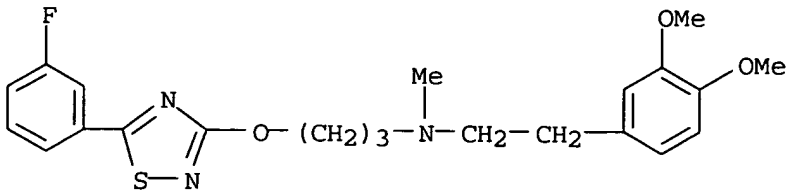
● HCl

RN 181938-16-9 HCAPLUS
CN Benzeneethanamine, N-[3-[[5-(4-fluorophenyl)-1,2,4-thiadiazol-3-yl]oxy]propyl]-3,4-dimethoxy-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



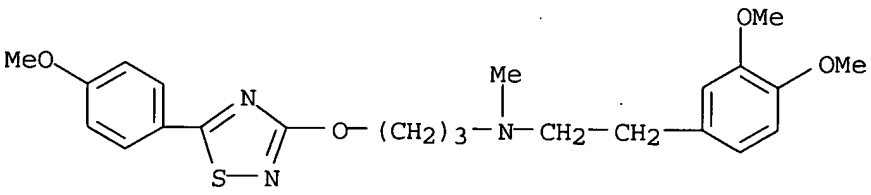
● HCl

RN 181938-19-2 HCAPLUS
CN Benzeneethanamine, N-[3-[[5-(3-fluorophenyl)-1,2,4-thiadiazol-3-yl]oxy]propyl]-3,4-dimethoxy-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



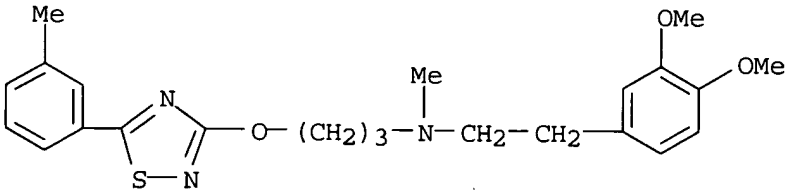
● HCl

RN 181938-22-7 HCAPLUS
CN Benzeneethanamine, 3,4-dimethoxy-N-[3-[[5-(4-methoxyphenyl)-1,2,4-thiadiazol-3-yl]oxy]propyl]-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



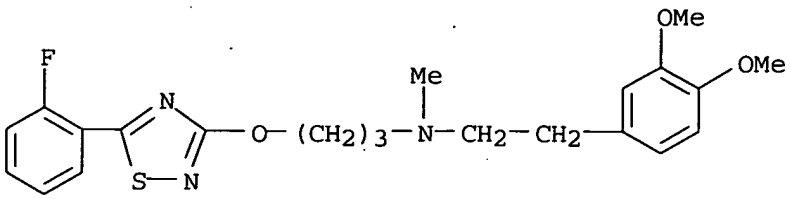
● HCl

RN 181938-25-0 HCAPLUS
CN Benzeneethanamine, 3,4-dimethoxy-N-methyl-N-[3-[[5-(3-methylphenyl)-1,2,4-thiadiazol-3-yl]oxy]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)



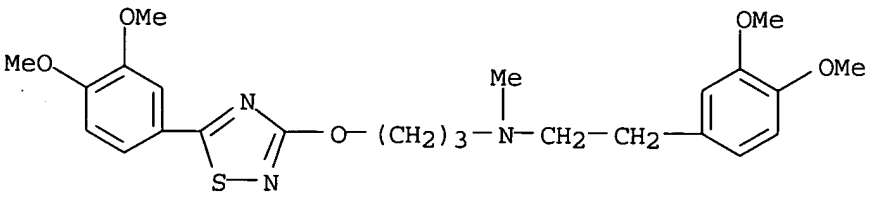
● HCl

RN 181938-28-3 HCAPLUS
CN Benzeneethanamine, N-[3-[[5-(2-fluorophenyl)-1,2,4-thiadiazol-3-yl]oxy]propyl]-3,4-dimethoxy-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



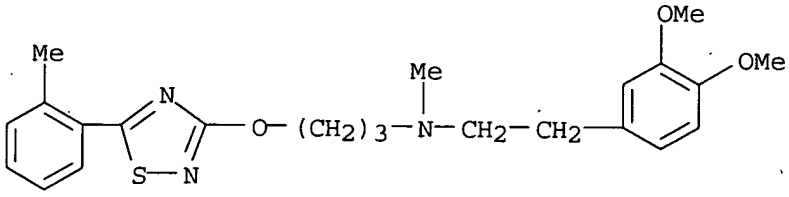
● HCl

RN 181938-34-1 HCAPLUS
CN Benzeneethanamine, N-[3-[[5-(3,4-dimethoxyphenyl)-1,2,4-thiadiazol-3-yl]oxy]propyl]-3,4-dimethoxy-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



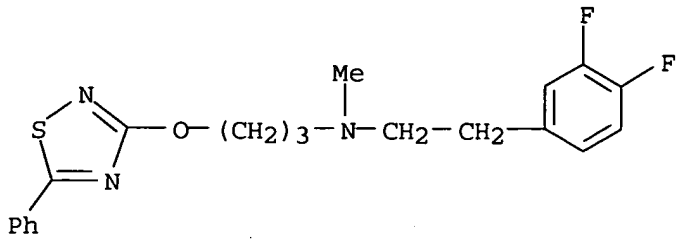
● HCl

RN 181938-39-6 HCAPLUS
CN Benzeneethanamine, 3,4-dimethoxy-N-methyl-N-[3-[[5-(2-methylphenyl)-1,2,4-thiadiazol-3-yl]oxy]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)



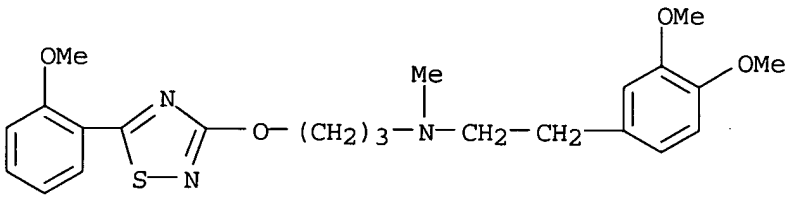
● HCl

RN 181938-41-0 HCAPLUS
CN Benzeneethanamine, 3,4-difluoro-N-methyl-N-[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)



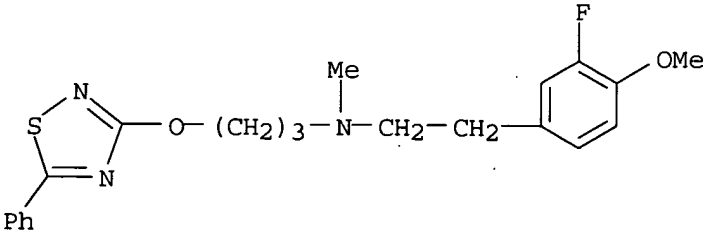
● HCl

RN 181938-43-2 HCAPLUS
CN Benzeneethanamine, 3,4-dimethoxy-N-[3-[[5-(2-methoxyphenyl)-1,2,4-thiadiazol-3-yl]oxy]propyl]-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



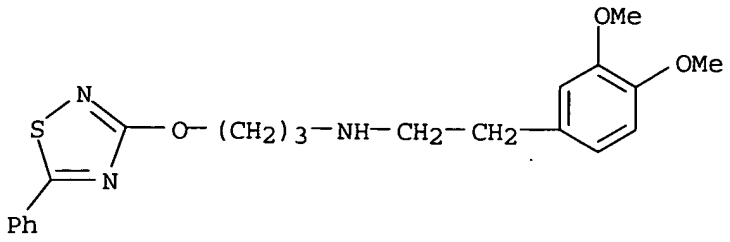
● HCl

RN 181938-45-4 HCAPLUS
CN Benzeneethanamine, 3-fluoro-4-methoxy-N-methyl-N-[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)



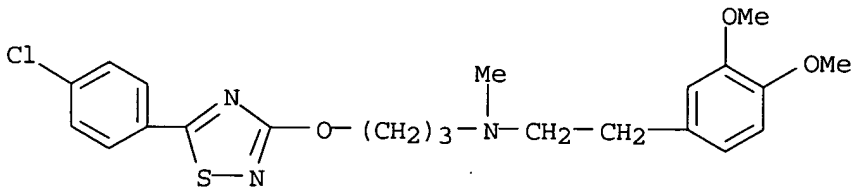
● HCl

RN 181938-50-1 HCAPLUS
CN Benzeneethanamine, 3,4-dimethoxy-N-[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)



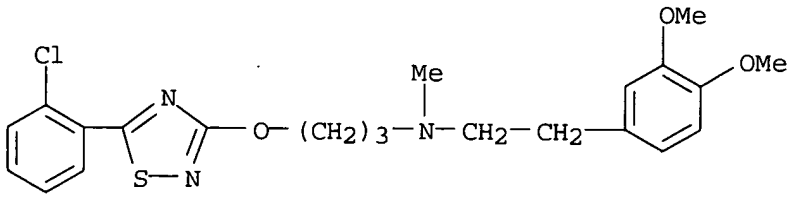
● HCl

RN 181938-57-8 HCAPLUS
CN Benzeneethanamine, N-[3-[[5-(4-chlorophenyl)-1,2,4-thiadiazol-3-yl]oxy]propyl]-3,4-dimethoxy-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



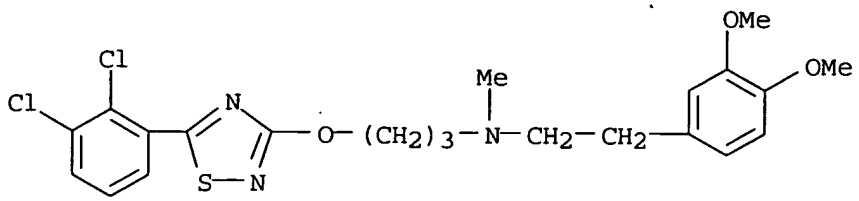
● HCl

RN 181938-59-0 HCAPLUS
CN Benzeneethanamine, N-[3-[[5-(2-chlorophenyl)-1,2,4-thiadiazol-3-yl]oxy]propyl]-3,4-dimethoxy-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



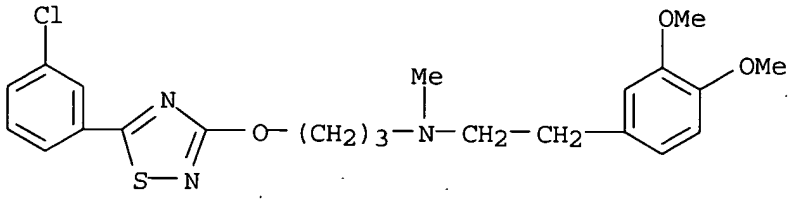
● HCl

RN 181938-60-3 HCAPLUS
CN Benzeneethanamine, N-[3-[[5-(2,3-dichlorophenyl)-1,2,4-thiadiazol-3-yl]oxy]propyl]-3,4-dimethoxy-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



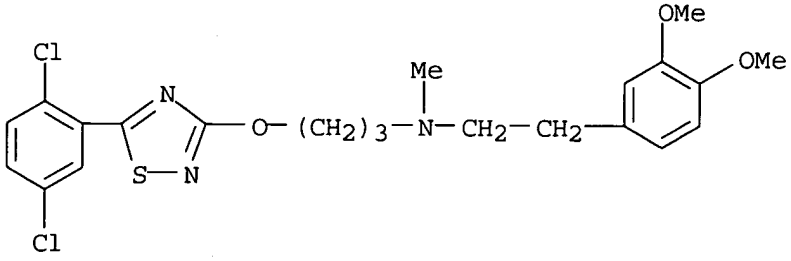
● HCl

RN 181938-61-4 HCAPLUS
CN Benzeneethanamine, N-[3-[[5-(3-chlorophenyl)-1,2,4-thiadiazol-3-yl]oxy]propyl]-3,4-dimethoxy-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



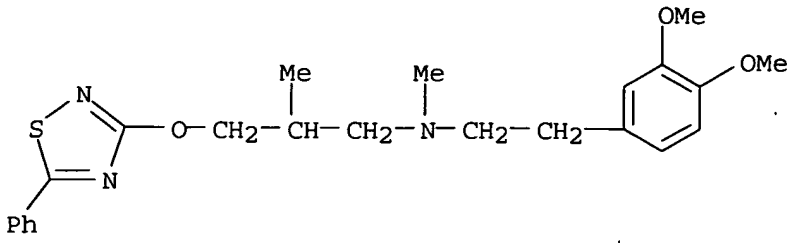
● HCl

RN 181938-64-7 HCAPLUS
CN Benzeneethanamine, N-[3-[[5-(2,5-dichlorophenyl)-1,2,4-thiadiazol-3-yl]oxy]propyl]-3,4-dimethoxy-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



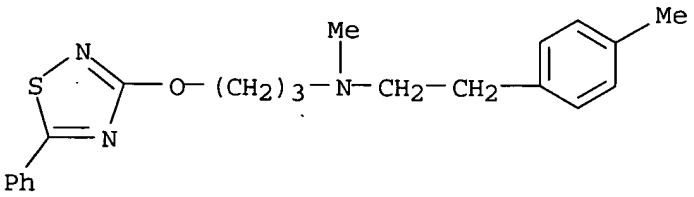
● HCl

RN 181938-66-9 HCAPLUS
CN Benzeneethanamine, 3,4-dimethoxy-N-methyl-N-[2-methyl-3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)



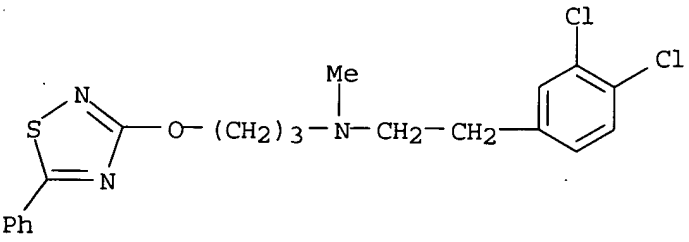
● HCl

RN 181938-71-6 HCAPLUS
CN Benzeneethanamine, N,4-dimethyl-N-[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)



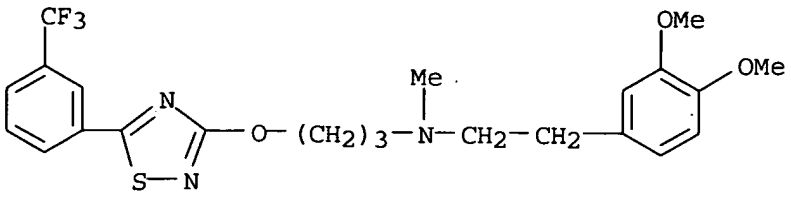
● HCl

RN 181938-73-8 HCAPLUS
CN Benzeneethanamine, 3,4-dichloro-N-methyl-N-[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)



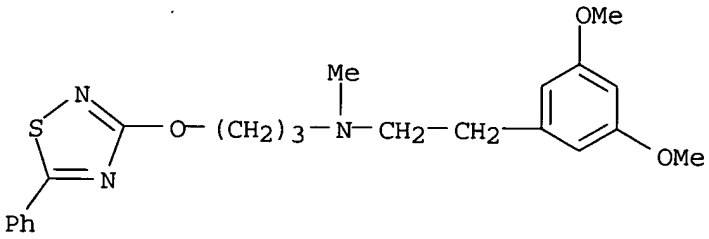
● HCl

RN 181938-75-0 HCAPLUS
CN Benzeneethanamine, 3,4-dimethoxy-N-methyl-N-[3-[[5-[3-(trifluoromethyl)phenyl]-1,2,4-thiadiazol-3-yl]oxy]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)

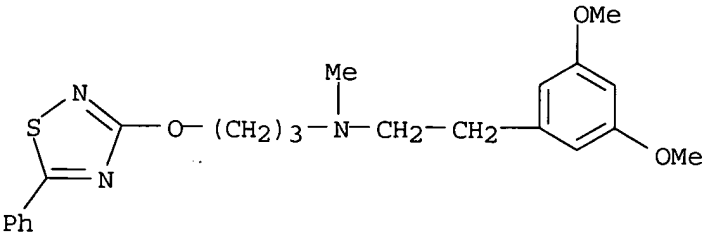


● HCl

RN 181954-84-7 HCAPLUS
CN Benzeneethanamine, 3,5-dimethoxy-N-methyl-N-[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]- (9CI) (CA INDEX NAME)

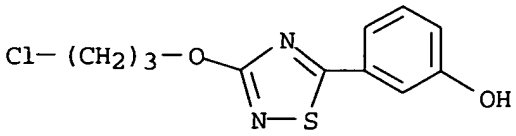


RN 181954-88-1 HCAPLUS
CN Benzeneethanamine, 3,5-dimethoxy-N-methyl-N-[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)

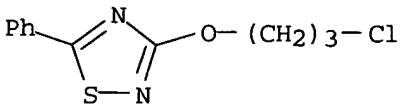


● HCl

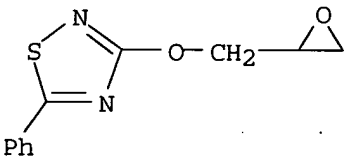
IT 181934-76-9P 181935-56-8P 181935-58-0P
181935-63-7P 181935-71-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
((phenylalkylaminoalkyloxy)-heteroaryl compds. having heart-rate-lowering and anti-ischemic effects)
RN 181934-76-9 HCAPLUS
CN Phenol, 3-[3-(3-chloropropoxy)-1,2,4-thiadiazol-5-yl]- (9CI) (CA INDEX NAME)



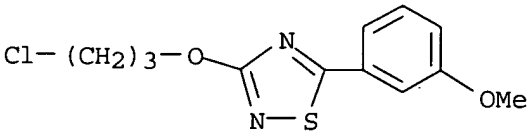
RN 181935-56-8 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(3-chloropropoxy)-5-phenyl- (9CI) (CA INDEX NAME)



RN 181935-58-0 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(oxiranylmethoxy)-5-phenyl- (9CI) (CA INDEX NAME)

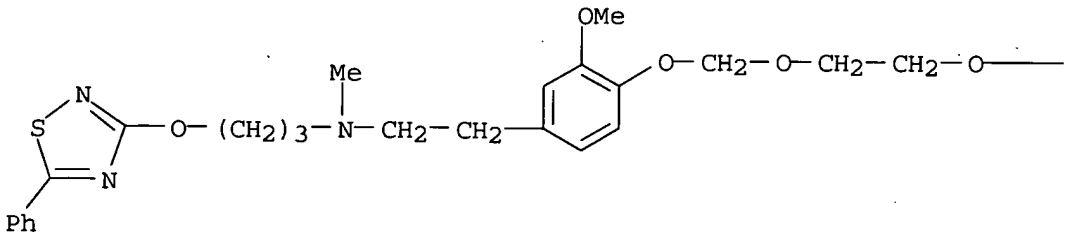


RN 181935-63-7 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(3-chloropropoxy)-5-(3-methoxyphenyl)- (9CI) (CA INDEX NAME)



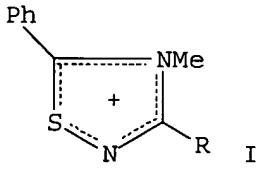
RN 181935-71-7 HCAPLUS
CN Benzeneethanamine, 3-methoxy-N-methyl-N-[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]-4-[[2-[(trimethylsilyl)oxy]ethoxy]methoxy]- (9CI) (CA INDEX NAME)

PAGE 1-A



—$SiMe_3$

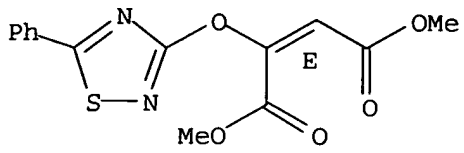
L11 ANSWER 9 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1984:174732 HCAPLUS
DOCUMENT NUMBER: 100:174732
TITLE: Cyclic meso-ionic compounds. Part 23. Novel chemistry of 1,2,4-thiadiazoles and their transformation into meso-ionic 1,2,4-thiadiazolium derivatives
AUTHOR(S): Newton, Christopher G.; Ollis, W. David; Wright, Derek E.
CORPORATE SOURCE: Dep. Chem., Univ. Sheffield, Sheffield, S3 7HT, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1984), (1), 75-84
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 100:174732
GI



I

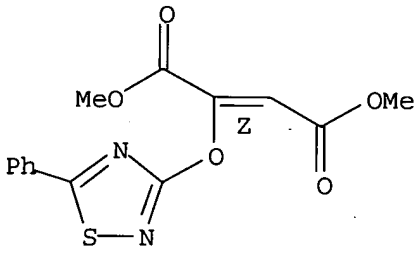
AB Mesoionic thiadiazolium compds. I (R = O-, N-SO2C6H4Me-4) were prepared by N-methylation of 3-hydroxy- and 3-(4-toluenesulfonamido)-5-phenyl-1,2,4-thiadiazole, resp. Reactions of 1,2,4-thiadiazoles with nucleophiles follow 2 general paths, reductive transformation to N-thiobenzoyl derivs. and elimination of S with formation of N-benzoyl derivs. A novel route to 1,2,4-thiadiazoles is described in which N-thiobenzoylureas and -guanidines are oxidized by bis(4-methoxyphenyl)telluroxide (II). E.g., treatment of N-methyl-N'-thiobenzoylurea with II in EtOH at room temperature for
30 min gave 84% 2-methyl-5-phenyl-1,2,4-thiadiazole-3(2H)-one.
IT 89879-89-0P 89879-90-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 89879-89-0 HCAPLUS
CN 2-Butenedioic acid, 2-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]-, dimethyl ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

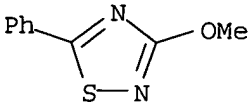


RN 89879-90-3 HCAPLUS
CN 2-Butenedioic acid, 2-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]-, dimethyl ester, (Z)- (9CI) (CA INDEX NAME)

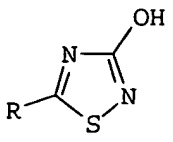
Double bond geometry as shown.



IT 89879-86-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by methylation of hydroxyphenylthiadiazole)
RN 89879-86-7 HCAPLUS
CN 1,2,4-Thiadiazole, 3-methoxy-5-phenyl- (6CI, 9CI) (CA INDEX NAME)



L11 ANSWER 10 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1980:6471 HCAPLUS
DOCUMENT NUMBER: 92:6471
TITLE: Effect of electrophilic reagents on the 3-hydroxy-1,2,4-thiadiazoles
AUTHOR(S): Taliani, Laurent; Perronnet, Jacques
CORPORATE SOURCE: Cent. Rech., Roussel-Uclaf, Romainville, 93230, Fr.
SOURCE: Journal of Heterocyclic Chemistry (1979), 16(5), 961-71
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: French
OTHER SOURCE(S): CASREACT 92:6471
GI



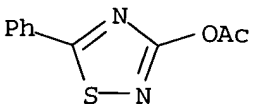
I

AB Electrophilic reagents may react either with the hydroxyl group in position 3, or with the 2-nitrogen atom of 3-hydroxy-1,2,4-thiadiazoles (I; R = alkoxy, alkylthio, NMe2). Hard electrophiles, such as acid chlorides, substitute on OH, whereas soft electrophiles (isocyanates, acid anhydrides) substitute on N.

IT 72183-12-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 72183-12-1 HCAPLUS

CN 1,2,4-Thiadiazol-3-ol, 5-phenyl-, acetate (ester) (9CI) (CA INDEX NAME)



L11 ANSWER 11 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1961:8056 HCAPLUS

DOCUMENT NUMBER: 55:8056

ORIGINAL REFERENCE NO.: 55:1587b-i,1588a-f

TITLE: Thiadiazoles. IX. Reactions of diazonium salts derived from 3-amino-1,2,4-thiadiazoles

AUTHOR(S): Kurzer, Frederick; Taylor, Sheila A.

CORPORATE SOURCE: Univ. London

SOURCE: Journal of the Chemical Society (1960) 3234-9
CODEN: JCSOA9; ISSN: 0368-1769

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

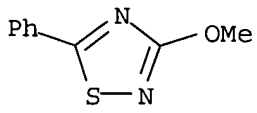
AB cf. CA 54, 4550a. 3-Halo- and 3-hydroxy-1,2,4-thiadiazoles were synthesized from the corresponding 3-amino compds. by way of the diazonium salts. Of the properties of the new 3-halo-1,2,4-thiadiazoles, their remarkable stability, and the relative inertness of the 3-halo substituent were noteworthy. 3-Amino-5-phenyl-1,2,4-thiadiazole (I) (7.08 g.) in 120 mL. concentrated HCl treated dropwise at -10 to -5° in the presence of a little Cu powder with 5.6 g. NaNO2 in 15 mL. H2O during 45 min., the suspension stirred 15 min. at -8°, 1-1.5 h. at room temperature, and finally 20 min. at 50-60°, diluted with 200 mL. H2O, stored at 0°, the crude solid collected, and extracted with ligroine gave residue A. Evaporation of the exts. gave 3.3-4.2 g. 3-chloro-5-phenyl-1,2,4-thiadiazole (II), yellow granules, m. 62-3° (ligroine). II was highly soluble in organic solvents except ligroine. The use of the inverted procedure gave 25% II as did expts. carried out without Cu powder. Residue A (2.5-5.5 g.) was partially fractionated as follows. (a) The residue (2.5 g.) from an experiment extracted at 50° with 30 and 15 mL. N NaOH, the filtered exts. acidified, and the precipitate collected gave 0.65 g. 3-hydroxy-5-phenyl-1,2,4-thiadiazole (III), m. 202-3° (decomposition)

(alc.). (b) The residue (5 g.) extracted with hot H2O deposited from the filtrates 1.8 g. solid, which extracted with hot alc. gave 1.1 g. benzoylurea, m. 211-13° (Me2CO-alc.). The alc. exts. afforded 0.4 g. III. II resisted hydrogenation at atmospheric pressure in the presence of Raney Ni and PtO2. It was unaffected when heated 3 h. at 100° with concentrated H2SO4 but was completely decomposed when refluxed 30 min. in 50% aqueous alc. and M KOH. The compound (70%) was recovered after treatment with MeNH2. II was destroyed by N2H4 and failed to react with p-toluenesulfonylhydrazine. II was not convertible into the 3-cyano compound by CuCN. It did not give the 3-thiol on treatment with CS(NH2)2-KOH (recovery 90%). An intimate mixture of 1.77 g. I and 3.45 g. NaNO2 was added in small portions during 0.5 h. to 35 mL. 35% HBr at -6 to -8° containing a little Cu powder, the suspension stirred 20 min. at -8°, allowed to reach room temperature during 1.5 h., finally heated at 50-5°, cooled, the mixture added to H2O, the oily layer (B) separated, and the aqueous phase extracted with Et2O. The oily layer B extracted with Et2O gave an orange ether solution and an unidentified olive-brown solid. The combined ether exts. evaporated and the residue extracted with ligroine gave a yellow gum. The extract afforded 0.52 g. 3-bromo-5-phenyl-1,2,4-thiadiazole (IV), yellow flakes, m. 64-6.6°. IV was also obtained in 12% yield by the procedure described for II but with 60% HBr. 3-Amino-5-anilino-1,2,4-thiadiazole (IVa) (solvate, 2.38 g.) and 3.45 g. NaNO2 added during 45 min. to 30 mL. concentrated HCl at -8°, the mixture worked up as described above, the product extracted with 70 mL. hot MeOH, evaporated, and the residue extracted with hot CHCl3 gave 0.15 g. 5-anilino-3-chloro-1,2,4-thiadiazole, m. 139-41° (50% aqueous alc.). 3-Amino-5-methylamino-1,2,4-thiadiazole p-toluenesulfonate (3.02 g.) in 30 mL. concentrated HCl containing Cu powder treated during 15 min. at -8° with 1.4 g. NaNO2, the mixture stirred 51 min. at -8°, at room temperature 0.5 h., and 15 min. at 50-60°, the suspension diluted with 50 mL. H2O, and extracted with Et2O and CHCl3 gave 5-7% 3-chloro-5-methylamino-1,2,4-thiadiazole (V), m. 132-4° (H2O). V was soluble in H2O. A number of attempts made to prepare 3-iodo-5-phenyl-1,2,4-thiadiazole by interaction of the appropriate diazonium salt solution with KI under various conditions were unsuccessful. The yellow liquid obtained on dissolving 1.77 g. I in 10 mL. concentrated H2SO4 treated successively at -8° with 0.76 g. NaNO2 in 10 mL. concentrated H2SO4 during 10 min. then with 10 mL. 80% H3PO4 during 1 h., 2 g. powdered CO(NH2)2 added during 5 min. and finally 1.7 g. KI in 2 mL. H2O-1 mL. 80% H3PO4 during 0.5 h., the mixture stirred 3 h. at room temperature, 100 g. ice added, the solid collected, washed, the residue dissolved in N NaOH, and the filtered extract acidified gave 0.68 g. III. Basification of the filtrate gave 0.4 g. starting material. II (0.49 g.) in 0.23 g. Na and 5 mL. MeOH refluxed 2 h. gave 0.33 g. 3-methoxy-5-phenyl-1,2,4-thiadiazole, m. 50-1° (ligroine). II (0.0025 mol) heated 1.5 h. with 0.01 g. atom Na in 4 mL. PhCH2OH at 80°, the mixture diluted with 0.015 mol 0.5N HCl, the PhCH2OH removed, the residual oil extracted with Et2O, the solvent removed, and the solid crystallized gave 0.36 g. 3-benzyloxy-5-phenyl-1,2,4-thiadiazole, m. 67-9° (ligroine). II (0.0025 mol) heated during 2 h. with 0.012 g. atom Na in 4 mL. (CH2OH)2, the mixture stirred into 50 mL. H2O, and the solidified oil crystallized gave 0.42 g. 3-(2-hydroxyethoxy)-5-phenyl-1,2,4-thiadiazole, m. 81-2° (ligroine-MeOH). I (1.77 g.) in 15 mL. concentrated H2SO4 and 15 mL. H2O diazotized at -10° by adding during 12 min. 1.04 g. NaNO2 in 4 mL. H2O, the mixture stirred a further 15-20 min. at -10°, the temperature raised during 0.5 h. to 25°, the liquid diluted with 25 mL. H2O, the suspension heated to 100°, and stored at 0° gave a solid;

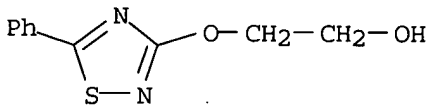
the solid dissolved in N NaOH and the solution acidified gave 1.04 g. III. III (0.45 g.) in 8 mL. Ac2O refluxed 20 min. gave 0.36 g. mono-Ac derivative, m. 141-2° (alc.). III (0.025 mol) in 5 mL. C5H5N treated during 15 min. at 100° with 0.7 g. BzCl gave 0.42 g. Bz derivative, yellow prisms, m. 73-5°. III with p-MeC6H4SO2Cl gave 81% mono-p-toluenesulfonate, needles, m. 93-4° (alc.). 3-Amino-5-(p-nitrophenyl)-1,2,4-thiadiazole (0.55 g.) in 5 mL. concentrated H2SO4 and 5 mL. H2O treated at -6 to -8° with 0.26 g. NaNO2 in 2 mL. H2O gave 0.18-0.24 g. 3-hydroxy-5-(p-nitrophenyl)-1,2,4-thiadiazole, orange granules, m. 251-3° (decomposition) (MeOH). Powdered NaNO2 (1.04 g.) added to 10 mL. cold concentrated H2SO4, the solution treated during 15 min. with 2.38 g. IVa in 10 mL. concentrated H2SO4 at -8 to -10°, the mixture stirred while 15 mL. 85% H3PO4 was added during 40 min., the mixture stirred 45 min. at -5°, poured into ice H2O, the mixture warmed 10 min. to 50°, filtered, the filtrate adjusted to pH 4, extracted with 80 mL. 40% NaOH, and the filtered solution acidified gave 0.72 g. 5-anilino-3-hydroxy-1,2,4-thiadiazole (VI), m. 207-8° (Me2CO-alc.). Acidification of the extract gave a small yield of crude unidentified material, m. between 152-9°. VI (0.5 g.) in 3 mL. POCl3 refluxed during 0.5 h. and the yellow liquid stirred into ice gave a resinous solid. Addition to the above mixture of 1 mL. PhNMe2 did not give more favorable results.

IT 89879-86-7, 1,2,4-Thiadiazole, 3-methoxy-5-phenyl-
99072-03-4, Ethanol, 2-(5-phenyl-1,2,4-thiadiazol-3-yloxy)-
108619-03-0, 1,2,4-Thiadiazole, 3-(benzyloxy)-5-phenyl-
(preparation of)

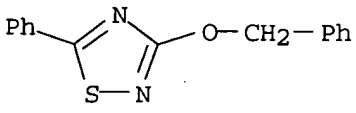
RN 89879-86-7 HCAPLUS
CN 1,2,4-Thiadiazole, 3-methoxy-5-phenyl- (6CI, 9CI) (CA INDEX NAME)



RN 99072-03-4 HCAPLUS
CN Ethanol, 2-(5-phenyl-1,2,4-thiadiazol-3-yloxy)- (6CI) (CA INDEX NAME)



RN 108619-03-0 HCAPLUS
CN 1,2,4-Thiadiazole, 3-(benzyloxy)-5-phenyl- (6CI) (CA INDEX NAME)



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